Learning through Experimentation
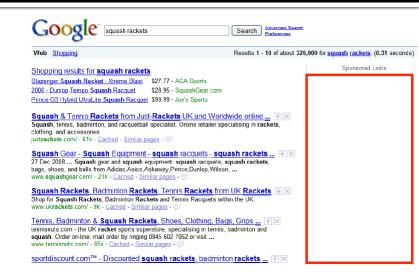
CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
http://cs246.stanford.edu

Learning through Experimentation
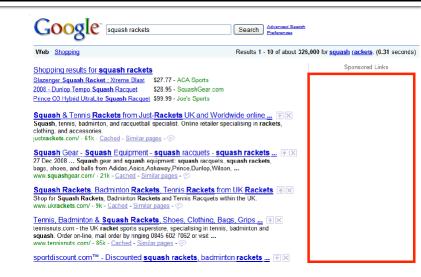
- **Web advertising**
  - We discussed how to match advertisers to queries in real-time
  - **But we did not discuss how to estimate the CTR (Click-Through Rate)**
- **Recommendation engines**
  - We discussed how to build recommender systems
  - **But we did not discuss the cold start problem**

Learning through Experimentation

- **What do CTR and cold start have in common?**
- **With every ad we show/product we recommend we gather more data about the ad/product**

- **Theme: Learning through experimentation**

Example: Web Advertising

- **Google's goal: Maximize revenue**
- **The old way: Pay by impression (CPM)**
  - **Best strategy: Go with the highest bidder**
    - But this ignores "effectiveness" of an ad
- **The new way: Pay per click! (CPC)**
  - **Best strategy: Go with expected revenue**
  - What's the expected revenue of ad **a for query q**?
  - $E[revenue_{a,q}] = P(click_a \mid q) * amount_{a,q}$

Prob. user will click on ad **a** given that she issues query **q**
(Unknown! Need to gather information)

Bid amount for ad **a** on query **q**
(Known)

Other Applications

- **Clinical trials:**
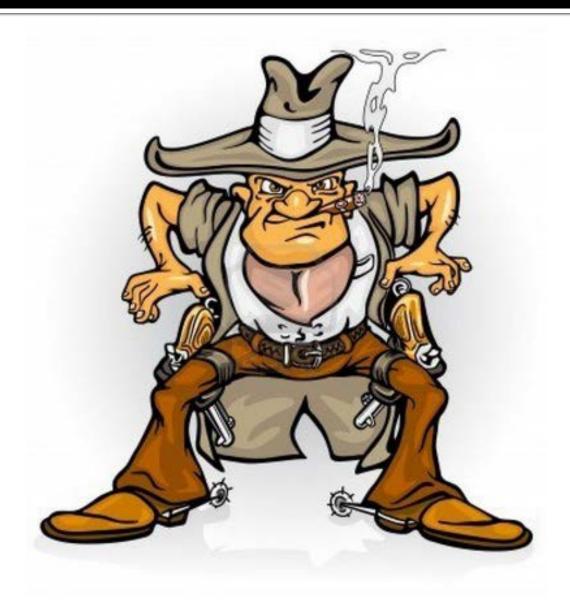 - Investigate effects of different treatments while minimizing patient losses
- **Adaptive routing:**
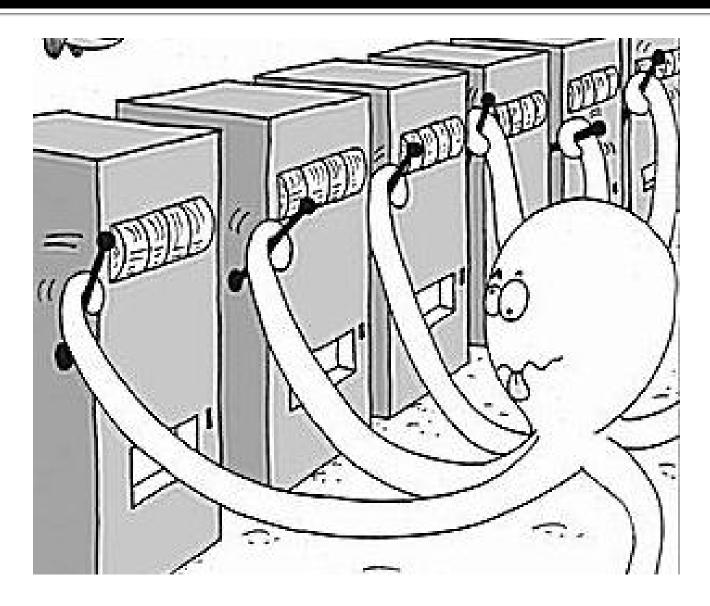 - Minimize delay in the network by investigating different routes
- **Asset pricing:**
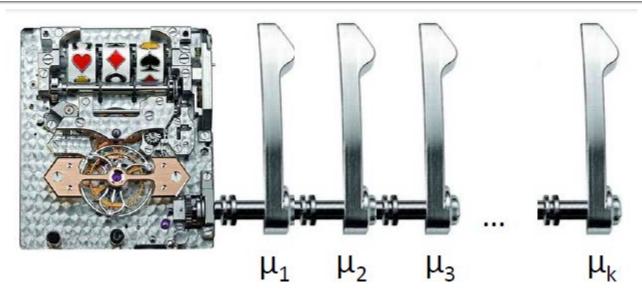 - Figure out product prices while trying to make most money

Approach: Bandits

Approach: Multiarmed Bandits

k-Armed Bandit

- **Each arm *a***
  - **Wins** (reward=**1**) with fixed (unknown) prob. μ_a
  - **Loses** (reward=**0**) with fixed (unknown) prob. $1-\mu_a$
- All draws are independent given $\mu_1 \ldots \mu_k$
- **How to pull arms to maximize total reward?**

k-Armed Bandit

μ_1 μ_2 μ_3 ... μ_k

- **How does this map to our setting?**
- Each **query** is a **bandit**
- Each **ad** is an **arm**
- **We want to estimate the arm's probability of winning μ_a (i.e., ad's the CTR μ_a)**
- Every time we pull an arm we do an 'experiment'

Stochastic k-Armed Bandit

The setting:

- Set of *k* choices (arms)
- Each choice *a* is associated with unknown probability distribution P_a supported in **[0,1]**
- We play the game for *T* rounds
- In each round *t*:
  - **(1)** We pick some arm *j*
  - **(2)** We obtain random sample X_t from P_j
    - Note reward is independent of previous draws
- **Our goal is to maximize** $\sum_{t=1}^{T} X_t$
- **But we don't know** μ_a**!** But every time we pull some arm *a* we get to learn a bit about μ_a

Online Optimization

- **Online optimization with limited feedback**

Choices	X_1	X_2	X_3	X_4	X_5	X_6	...
a_1					1	1	
a_2	0		1	0			
...							
a_k		0					

Time →

- **Like in online algorithms:**

  - **Have to make a choice each time**

  - **But we only receive information about the chosen action**

Solving the Bandit Problem

- **Policy**: a strategy/rule that in each iteration tells me which arm to pull
  - Hopefully policy depends on the history of rewards

- **How to quantify performance of the algorithm? Regret!**

Performance Metric: Regret

- Let be μ_a the mean of P_a
- Payoff/reward of **best arm**: $\mu^* = \max\limits_a \mu_a$
- Let $i_1, i_2 \ldots i_T$ be the sequence of arms pulled
- Instantaneous **regret** at time t: $r_t = \mu^* - \mu_{a_t}$
- **Total regret:**

$$R_T = \sum_{t=1}^{T} r_t$$

- **Typical goal: Want a policy (arm allocation strategy) that guarantees:** $\frac{R_T}{T} \to 0$ as $T \to \infty$

Allocation Strategies

- **If we knew the payoffs, which arm would we pull?**

$$\text{Pick} \quad \arg\max_a \mu_a$$

- **What if we only care about estimating payoffs μ_a?**

  - Pick each of k arms equally often: $\frac{T}{k}$

  - **Estimate:** $\widehat{\mu_a} = \frac{k}{T} \sum_{j=1}^{T/k} X_{a,j}$

  - **Regret:** $R_T = \frac{T}{k} \sum_a^k (\mu^* - \mu_a)$

Bandit Algorithm: First try

- **Regret is defined in terms of average reward**
- **So, if we can estimate avg. reward we can minimize regret**
- **Consider algorithm: *Greedy*
  Take the action with the highest avg. reward**
  - **Example:** Consider 2 actions
    - **A1** reward 1 with prob. 0.3
    - **A2** has reward 1 with prob. 0.7
  - Play **A1**, get reward 1
  - Play **A2**, get reward 0
  - Now avg. reward of **A1** will never drop to 0, and we will never play action **A2**

Exploration vs. Exploitation

- **The example illustrates a classic problem in decision making:**
  - We need to trade off **exploration** (gathering data about arm payoffs) and **exploitation** (making decisions based on data already gathered)

- **The Greedy does not explore sufficiently**
  - **Exploration:** Pull an arm we never pulled before
  - **Exploitation:** Pull an arm a for which we currently have the highest estimate of μ_a

Optimism

- The problem with our **Greedy** algorithm is that it is **too certain** in the estimate of μ_a
    - When we have seen a single reward of 0 we shouldn't conclude the average reward is 0

- **Greedy does not explore sufficiently!**

New Algorithm: Epsilon-Greedy

Algorithm: Epsilon-Greedy

- **For t=1:T**

  - Set $\varepsilon_t = O(1/t)$

  - **With prob. ε_t: Explore** by picking an arm chosen uniformly at random

  - **With prob. $1 - \varepsilon_t$: Exploit** by picking an arm with highest empirical mean payoff

- **Theorem** [Auer et al. '02]

  For suitable choice of ε_t it holds that

$$R_T = O(k \log T) \Rightarrow \frac{R_T}{T} = O\left(\frac{k \log T}{T}\right) \to 0$$

Issues with Epsilon Greedy

- What are some issues with **Epsilon Greedy**?
  - **"Not elegant"**: Algorithm explicitly distinguishes between exploration and exploitation

  - **More importantly:** Exploration makes **suboptimal choices** (since it picks any arm equally likely)

- **Idea:** When exploring/exploiting we need to **compare** arms

Comparing Arms

- **Suppose we have done experiments:**
  - **Arm 1**: 1 0 0 1 1 0 0 1 0 1
  - **Arm 2**: 1
  - **Arm 3**: 1 1 0 1 1 1 0 1 1 1
- **Mean arm values:**
  - **Arm 1**: 5/10, **Arm 2**: 1, **Arm 3**: 8/10

- **Which arm would you pick next?**

- **Idea:** **Don't just look at the mean (that is, expected payoff) but also the confidence!**
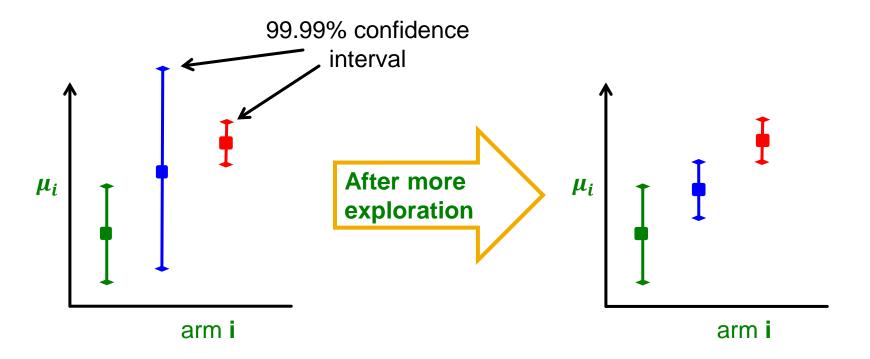
Confidence Intervals (1)

- **A confidence interval is a range of values within which we are sure the mean lies with a certain probability**

  - We could believe μ_a is within [0.2,0.5] with probability 0.95

  - If we would have tried an action less often, our estimated reward is less accurate so the confidence interval is larger

  - Interval shrinks as we get more information (try the action more often)

Confidence Intervals (2)

- **Assuming we know the confidence intervals**

- **Then, instead of trying the action with the highest mean we can try the action with the highest upper bound on its confidence interval**

- This is called an **optimistic policy**
  - We believe an action is as good as possible given the available evidence

Confidence Based Selection

99.99% confidence interval

After more exploration

arm **i**

arm **i**

Calculating Confidence Bounds

Suppose we fix arm a:

- Let $Y_{a,1} \ldots Y_{a,m}$ be the payoffs of arm a in the first m trials
  - So, $Y_{a,1} \ldots Y_{a,m}$ are **i.i.d.** rnd. vars. taking values in **[0,1]**
- **Mean payoff of arm a: $\mu_a = E[Y_{a,m}]$**
- **Our estimate: $\widehat{\mu_{a,m}} = \frac{1}{m} \sum_{\ell=1}^{m} Y_{a,\ell}$**
- Want to find b such that with high probability $\left| \mu_a - \widehat{\mu_{a,m}} \right| \leq b$
  - Also want b to be as small as possible (**why?**)

- **Goal: Want to bound** $P\left(\left| \mu_i - \widehat{\mu_{a,m}} \right| \leq b \right)$
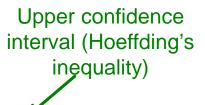
Hoeffding's Inequality

- **Hoeffding's inequality:**
  - Let $X_1 \ldots X_m$ be **i.i.d.** rnd. vars. taking values in **[0,1]**
  - Let $\mu = E[X]$ and $\widehat{\mu_m} = \frac{1}{m}\sum_{\ell=1}^{m} X_\ell$
  - **Then:** $P(|\mu - \widehat{\mu_m}| \leq b) \leq 2\,exp(-2b^2 m) = \delta$

- **To find out the confidence interval b (for a given confidence level δ) we solve**
  - $2e^{-2b^2 m} \leq \delta$ **then** $-2b^2 m \leq \ln(\delta/2)$

  - **So:** $b \geq \sqrt{\dfrac{\ln\left(\frac{2}{\delta}\right)}{2\,m}}$

UCB1 Algorithm

- **UCB1 (Upper confidence sampling) algorithm**
  - **Set: $\widehat{\mu}_1 = \cdots = \widehat{\mu}_k = 0$ and $m_1 = \cdots = m_k = 0$**
    - **$\widehat{\mu}_a$ is our estimate of payoff of arm i**
    - **m_a is the number of pulls of arm i so far**
  - **For $t = 1:T$**

    Upper confidence interval (Hoeffding's inequality)

    - **For each arm a calculate: $UCB(a) = \widehat{\mu}_a + \alpha\sqrt{\dfrac{2\ln t}{m_a}}$**
    - **Pick arm $j = arg\ max_a\ UCB(a)$**
    - **Pull arm j and observe y_t**
    - **Set: $m_j \leftarrow m_j + 1$ and $\widehat{\mu}_j \leftarrow \dfrac{1}{m_j}\left(y_t + (m_j - 1)\widehat{\mu}_j\right)$**

UCB1: Discussion

$$UCB(a) = \widehat{\mu_a} + \alpha \sqrt{\frac{2 \ln t}{m_a}}$$

$$b \geq \sqrt{\frac{\ln\left(\frac{2}{\delta}\right)}{2\,m}}$$

- Confidence interval **grows** with the total number of actions t we have taken

- But **shrinks** with the number of times m_a we have tried arm a

- This ensures each arm is tried infinitely often but still balances exploration and exploitation

- α plays the role of δ: $\alpha = f\left(\frac{2}{\delta}\right)$ $\qquad \alpha = 1 + \sqrt{\ln(2/\delta)/2}$

- **Optimism in face of uncertainty**

  - The algorithm believes that it can obtain extra rewards by reaching the unexplored parts of the state space

Performance of UCB1

- **Theorem [Auer et al. 2002]**
  - Suppose optimal mean payoff is $\boldsymbol{\mu}^* = \max_{\boldsymbol{a}} \boldsymbol{\mu_a}$

  - And for each arm let $\boldsymbol{\Delta_a} = \boldsymbol{\mu}^* - \boldsymbol{\mu_a}$

  - **Then it holds that**

$$E[R_T] = \left[8 \sum_{a:\mu_a < \mu^*} \frac{\ln T}{\Delta_a} \right] + \left(1 + \frac{\pi^2}{3} \right) \left(\sum_{i=a}^{k} \Delta_a \right)$$

$$\boldsymbol{O(k \ln T)} \qquad\qquad \boldsymbol{O(k)}$$

  - **So:** $\boldsymbol{O\left(\dfrac{R_T}{T} \right) = k \, \dfrac{ln\,T}{T}}$

Summary so far

- **k**-armed bandit problem as a formalization of the exploration-exploitation tradeoff

- Analog of online optimization (e.g., SGD, BALANCE), but with **limited feedback**

- **Simple algorithms are able to achieve no regret (in the limit)**
  - Epsilon-greedy
  - UCB (Upper Confidence Sampling)

Back to News Recommendation

- **Every round receive context** [Li et al., WWW '10]
  - **Context:** User features, articles view before
- **Model for each article's click-through rate**

News Recommendation

- **Feature-based exploration:**

  - **Select articles to serve users based on contextual information about the user and the articles**

  - **Simultaneously adapt article selection strategy based on user-click feedback to maximize total number of user clicks**

Contextual Bandits

- **Contextual bandit algorithm in round t**

  - **(1) Algorithm** observes user u_t and a set A of arms together with their features $x_{t,a}$

    - Vector $x_{t,a}$ summarizes both the user u_t and arm a

    - We call vector $x_{t,a}$ the **context**

  - **(2)** Based on payoffs from previous trials, algorithm chooses arm $a \in A$ and receives payoff $r_{t,a}$

    - **Note only feedback for the chosen a is observed**

  - **(3)** Algorithm improves arm selection strategy with each observation $(x_{t,a}, a, r_{t,a})$

LinUCB Algorithm (1)

- Payoff of arm $\boldsymbol{a}$: $E\left[r_{t,a}|x_{t,a}\right] = x_{t,a}^{\mathrm{T}} \cdot \theta_a^*$

  - $\boldsymbol{x_{t,a}}$ ... $\boldsymbol{d}$-dimensional feature vector

  - $\boldsymbol{\theta_a^*}$... unknown coefficient vector we aim to learn

    - Note that $\boldsymbol{\theta_a^*}$ are not shared between different arms!

- **What's the difference between LinUCB, UCB1?**

  - UCB2 directly estimates $\boldsymbol{\mu_a}$ through experimentation (without any knowledge about arm $\boldsymbol{a}$)

  - LinUCB estimates $\boldsymbol{\mu_a}$ by regression $\boldsymbol{\mu_a = x_{t,a}^T \cdot \theta_a^*}$

    - The hope is that we will be able to learn faster as we consider the context $\boldsymbol{x_a}$ (user, ad) of arm $\boldsymbol{a}$

LinUCB Algorithm (2)

- Payoff of arm $\boldsymbol{a}$: $E\left[r_{t,a}|x_{t,a}\right] = x_{t,a}^{\mathrm{T}} \cdot \theta_a^*$
  - $\boldsymbol{x_{t,a}}$ ... $\boldsymbol{d}$-dimensional feature vector
  - $\boldsymbol{\theta_a^*}$... unknown coefficient vector we aim to learn

- **How to estimate θ_a?**
  - $\boldsymbol{D_a}$... $m \times d$ matrix of $\boldsymbol{m}$ training inputs $[\boldsymbol{x_{a,t}}]$
  - $\boldsymbol{b_a}$... $\boldsymbol{m}$-dim. vector of responses to $\boldsymbol{a}$ (click/no-click)
  - **Linear regression solution to θ_a is then**
    - $\widehat{\boldsymbol{\theta}}_a = \arg\min_{\boldsymbol{\theta}} \sum_{\boldsymbol{m} \in \boldsymbol{D_a}} \left(x_{t,a}^{\mathrm{T}} \cdot \theta_a - \boldsymbol{b_a^{(m)}} \right)^2$
      - Which is solved by: $\hat{\theta}_a = \left(D_a^{\mathrm{T}} D_a + I_d \right)^{-1} D_a^T b_a$

I$_d$ is **d** x **d** identity matrix

LinUCB Algorithm (3)

- **One can then show (using similar techniques as we used for UCB) that**

$$\left| \mathbf{x}_{t,a}^{\top} \hat{\boldsymbol{\theta}}_a - \mathbf{E}[r_{t,a}|\mathbf{x}_{t,a}] \right| \le \alpha \sqrt{\mathbf{x}_{t,a}^{\top}(\mathbf{D}_a^{\top}\mathbf{D}_a + \mathbf{I}_d)^{-1}\mathbf{x}_{t,a}}$$

$$\alpha = 1 + \sqrt{\ln(2/\delta)/2}$$

- **So LinUCB arm selection rule is:**

$$a_t \overset{\text{def}}{=} \arg\max_{a \in \mathcal{A}_t} \left(\mathbf{x}_{t,a}^{\top}\hat{\boldsymbol{\theta}}_a + \alpha \sqrt{\mathbf{x}_{t,a}^{\top}\mathbf{A}_a^{-1}\mathbf{x}_{t,a}} \right)$$

Estimated $\boldsymbol{\mu}_a$

Confidence interval:
Standard deviation

$$\mathbf{A}_a \overset{\text{def}}{=} \mathbf{D}_a^{\top}\mathbf{D}_a + \mathbf{I}_d$$

LinUCB Algorithm (3)

$$\mathbf{A}_a \stackrel{\text{def}}{=} \mathbf{D}_a^\top \mathbf{D}_a + \mathbf{I}_d$$

Initialization:

For each arm a:

$A_a = I_d$ identity matrix m x m

$b_a = [0]_d$ vector of zeros

Online algorithm:

For t = 1, 2, 3,… T:

Observe features of all arms $a : x_{t,a} \in R^d$

For each arm a:

$\theta_a = A_a^{-1} b_a$ regression coefficients

$p_{t,a} = \theta_a^T x_{t,a} + \alpha \sqrt{x_{t,a}^T A_a^{-1} x_{t,a}}$ confidence bound

Choose arm $a_t = \arg\max_a p_{t,a}$ choose arm

$A_{a_t} = A_{a_t} + x_{t,a_t} x_{t,a_t}^T$ update A for the chosen arm a_t

$b_{a_t} = b_{a_t} + r_t\, x_{t,a_t}$ updated b for the chosen arm a_t
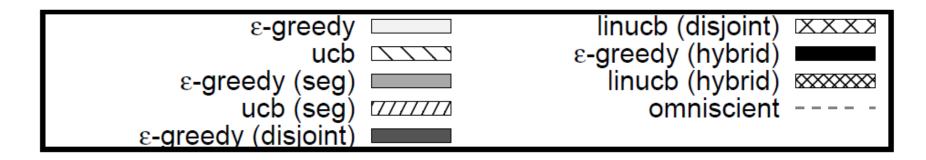
LinUCB: Discussion

- **LinUCB** computational complexity is
    - **Linear** in the **number of arms** and
    - At most **cubic** in the **number of features**

- **LinUCB** works well for a **dynamic arm set** (arms come and go):
    - For example, in news article recommendation, for instance, editors add/remove articles to/from a pool
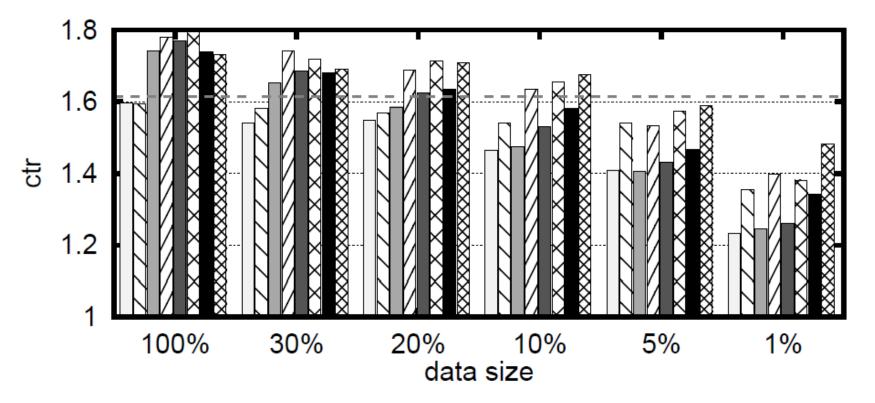
Yahoo! News Experiment

- **What to put in slots F1, F2, F3, F4 to make the user click?**

Results

Relevance vs. Diversity

- **Want to choose a set that caters to as many users as possible**

- **Users may have different interests, queries may be ambiguous**

- **Want to optimize both the relevance and diversity**

Announcement:
Final Exam Logistics

Final: At Stanford

- **Alternate final:**
  Tue 3/14 7:00-10:00pm in Cubberly Auditorium
    - Register here: http://bit.ly/Zsrigo
        - We have 100 slots. First come first serve!
- **Final: Mon 3/17 12:15-3:15pm in NVidia (lastname starting with A-J), GatesB01 (K-S), and Packard 101 (T-Z)**
    - **See** http://campus-map.stanford.edu
    - **Practice finals are posted on Piazza!**

- **SCPD students can take the exam at Stanford!**

Final: SCPD Students

- **Exam protocol for SCPD students:**

  - On Friday 3/14 your exam proctor will receive the PDF of the final exam from SCPD

  - **If you take the exam at Stanford:**
    - Ask the exam monitor to delete the SCP email

  - **If you don't take the exam at Stanford:**
    - Arrange **3h** slot with your exam monitor
    - You can take the exam **anytime** but return it in time
    - **Email exam PDF to cs246.mmds@gmail.com by Tuesday 3/15 11:59pm Pacific time**