

Model Counting for Logical Theories

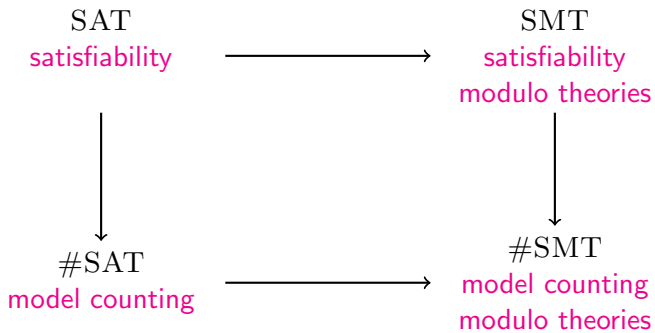
Wednesday

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Agenda

Tuesday computational complexity, probability theory

Wednesday randomized algorithms, Monte Carlo methods

Thursday hashing-based approach to model counting

Friday from discrete to continuous model counting

Outline

1. Randomized algorithms
Complexity classes **RP** and **BPP**
2. Monte Carlo methods
3. Markov chain Monte Carlo

Decision problems and algorithms

Decision problem:

$L \subseteq \{0, 1\}^*$ (encodings of yes-instances)

Algorithm for L :

says “yes” on every $x \in L$, “no” on every $x \in \{0, 1\}^* \setminus L$

Complexity classes: brief summary

P: polynomial time (efficiently solvable)

NP: nondeterministic polynomial time (with efficiently verifiable solutions)

#P: counting polynomial time

Examples of randomized algorithms

- ▶ Primality testing
- ▶ Polynomial identity testing
- ▶ Undirected reachability
- ▶ Volume estimation

Randomized algorithms: our model

The algorithm can toss fair coins:

1. Syntactically, a randomized algorithm is an algorithm that has access to a source of randomness, but acts deterministically if the random input is fixed.
2. It has on-demand access to arbitrary many independent random variables that have Bernoulli($\frac{1}{2}$) distribution.
3. Each request takes 1 computational step.

Deterministic and randomized time complexity

Recall **deterministic** time complexity:

- ▶ of algorithm \mathcal{A} on input x

Randomized time complexity:

Maximum (worst-case) over all possible sequences of random bits

Then take maximum (worst-case) over all inputs of length n .

Complexity classes **P**, **RP**, and **BPP**

P: class of languages L for which there exists a deterministic polynomial-time algorithm \mathcal{A} such that

$x \in L \implies \mathcal{A}(x)$ accepts

$x \notin L \implies \mathcal{A}(x)$ rejects

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RP: class of languages L for which there exists a randomized polynomial-time algorithm \mathcal{A} such that

$$x \in L \implies \text{P}[\mathcal{A}(x) \text{ accepts}] \geq 1/2$$

$$x \notin L \implies \text{P}[\mathcal{A}(x) \text{ accepts}] = 0$$

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Complexity classes **P**, **RP**, and **BPP**

Intuition:

P: deterministic polynomial time

RP: randomized polynomial time with one-sided error

BPP: randomized polynomial time with bounded two-sided error

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Definition of \mathbf{RP} via certificates

Recall: $L \in \mathbf{NP} \iff$

there exist a polynomial $p(n)$ and a polynomial-time algorithm $V(x, y)$ such that the following holds:

$x \in L \implies$ there exists a $y \in \{0, 1\}^{p(|x|)}$ such that $V(x, y) = \text{YES}$

$x \notin L \implies$ there is no such $y \in \{0, 1\}^{p(|x|)}$

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there exists a polynomial $p(n)$ and a polynomial-time algorithm $V(x, y)$ such that the following holds:

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Hence, $\mathbf{RP} \subseteq \mathbf{NP}$.

Definition of **BPP** via certificates

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Error reduction (confidence amplification) for **RP**

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Error reduction:

- ▶ Can replace $1/2$ above with $1 - 2^{-n^d}$ for any $d \geq 1$.
- ▶ Can replace $1/2$ above with $1/n^d$ for any $d \geq 1$.

Error reduction (confidence amplification) for **BPP**

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Error reduction:

- ▶ Can replace $\frac{1}{4}$ above with 2^{-n^d} for any $d \geq 1$.
- ▶ Can replace $\frac{1}{4}$ above with $\frac{1}{2} - 1/n^d$ for any $d \geq 1$.

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Model counting and probability

Recall:

The model count of a formula $\varphi(x_1, \dots, x_k)$ is $\text{mc}(\varphi) = \mu(\llbracket \varphi \rrbracket)$.

A logical theory \mathcal{T} is measured if every $\llbracket \varphi \rrbracket$ is measurable.

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Suppose $\llbracket\varphi\rrbracket \subseteq D^k$, and assume $\mu(D) < \infty$.

Let \mathcal{F} be the σ -algebra of measurable subsets of D^k .

Then $P: \mathcal{F} \rightarrow [0, 1]$ given by

$$P(A) = \frac{\mu(A)}{\mu(D^k)}$$

is a probability measure on D^k .

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Then $\text{mc}(\varphi) = P(\llbracket\varphi\rrbracket) \cdot \mu(D^k)$.

Model counting via estimation of probability

The equality

$$\text{mc}(\varphi) = P(\llbracket \varphi \rrbracket) \cdot \mu(D^k)$$

reduces model counting to computing the probability of an event.

Probability estimation

Suppose we are given (implicitly) a probability space (Ω, \mathcal{F}, P) .

Our goal is to estimate the value of $P(A)$.

Probability estimation via sampling

In order to estimate $P(A)$, we can observe multiple independent copies of the indicator variable $\mathbf{1}_A$ where $A \in \mathcal{F}$.

This corresponds to random sampling and checking whether the event A has occurred.

Equivalently, we observe multiple independent random variables that have Bernoulli distribution with parameter $\theta = P(A)$.

Our goal is to estimate θ given the observations.

The mean as the estimate

Given the values of X_1, \dots, X_n in $\{0, 1\}$, the unknown parameter θ should be close to

$$\bar{X} = \frac{X_1 + \dots + X_n}{n}.$$

Why?

The mean as the estimate

Given the values of X_1, \dots, X_n in $\{0, 1\}$, the unknown parameter θ should be close to

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Why?

$$\begin{aligned} \mathbb{E} \bar{X} &= \mathbb{E} \frac{X_1 + \dots + X_n}{n} = \frac{\mathbb{E} X_1 + \dots + \mathbb{E} X_n}{n} \\ &= \frac{\theta + \dots + \theta}{n} = \theta \end{aligned}$$

By Chebyshev's inequality, only rarely does \bar{X} take values away from $\mathbb{E} X = \theta$.

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Is that sufficient?

Approximation

We want to estimate a certain quantity f .

Suppose our estimate is $\tilde{f} = \tilde{f}(\varepsilon)$,
where ε is an input parameter.

Additive error:

$$|\tilde{f}(\varepsilon) - f| \leq \varepsilon$$

Multiplicative error:

$$|\tilde{f}(\varepsilon) - f| \leq \varepsilon \cdot f$$

Randomized approximation

We want to estimate a certain quantity f .

Suppose our estimate is $\tilde{f} = \tilde{f}(\varepsilon, \alpha)$,
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$$\mathbb{P}[|\tilde{f}(\varepsilon, \alpha) - f| \leq \varepsilon] \geq 1 - \alpha$$

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We want to find **efficient** randomized approximation schemes.

The mean as the estimate

Given the values of X_1, \dots, X_n in $\{0, 1\}$, the unknown parameter θ should be close to

$$\bar{X} = \frac{X_1 + \dots + X_n}{n}.$$

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Estimates from the Chebyshev bound

Chebyshev inequality:

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$n \geq \frac{1}{4\alpha\varepsilon^2}$ samples are sufficient

for additive error ε and confidence parameter α

Estimates from the Chernoff bound

Chernoff bound:

$$P(|\bar{X} - EX| \geq t) \leq 2 \exp(-nt^2/4)$$

if X_1, \dots, X_n are independent and identically distributed in $[0, 1]$

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if X_1, \dots, X_n are independent and identically distributed in $[0, 1]$

$n \geq \frac{4}{\ln(2/\alpha)\varepsilon^2}$ samples are sufficient

for additive error ε and confidence parameter α

Conclusion: Model counting via Monte Carlo

Algorithm:

1. Given a formula $\varphi(x_1, \dots, x_k)$, sample uniformly from possible models.
2. Return the proportion of actual models times $\mu(D^k)$.

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The Knapsack Problem revisited

Consider the counting version of the Knapsack problem.

Given $a_1, \dots, a_n \in \mathbb{N}$ and $b \in \mathbb{N}$, **compute the number** N of vectors $(x_1, \dots, x_n) \in \{0, 1\}^n$ that satisfy $\sum_{i=1}^n a_i x_i \leq b$.

This problem is **#P**-complete.

A Monte Carlo algorithm for Knapsack

$C = 0$

For $k = 1, \dots, m$

1. Sample (x_1, \dots, x_n) uniformly at random from $\{0, 1\}^n$.
2. If $\sum_{i=0}^n a_i x_i \leq b$ then $C = C + 1$.

Return $Y = \binom{C}{m} 2^n$

Y is the random variable corresponding to the output. $E(Y) = N$.

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Return $Y = \left(\frac{C}{m}\right)2^n$

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We can make m sufficiently large to obtain a reliable approximation with any desired accuracy.

What's the problem?

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Y is the random variable corresponding to the output. $E(Y) = N$.

Let Z_k be random variable such that $Z_k = 1$ if $\sum_{i=1}^n a_i x_i \leq b$ at the k -th iteration and $Z_k = 0$ otherwise.

Z_1, Z_2, \dots are independent Bernoulli random variables with parameter $p = \frac{N}{2^n}$. Let \bar{Z} be the number of failures before the first success. \bar{Z} has geometric distribution with parameter p . Thus,

$$E\bar{Z} = \frac{1-p}{p} = \frac{1}{p} - 1 = \frac{2^n}{N} - 1.$$

If N is sub-exponential (e.g., polynomial in n), we need an **exponential number of steps** before the first success!

An alternative?

Sample from the uniform distribution over the set of solutions

$$\Omega_{\text{KNAPSACK}} = \{(x_1, \dots, x_n) \in \{0, 1\}^n : \sum_{i=0}^n a_i x_i \leq b\}.$$

How? Use a **Markov chain Monte Carlo** method.

Markov Chains: Definition

Finite Markov chain $\mathfrak{M} = (\Omega, T)$

- ▶ finite set of states Ω ,
- ▶ transition probability matrix T where

$$T_{s,s'} = \text{P}(\text{next state will be } s' \mid \text{the current state is } s)$$

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A Markov chain $\mathfrak{M}_{\text{KNAPSACK}} = (\Omega_{\text{KNAPSACK}}, T_{\text{KNAPSACK}})$ for Knapsack

- ▶ $\Omega_{\text{KNAPSACK}} = \{(x_1, \dots, x_n) \in \{0, 1\}^n : \sum_{i=1}^n a_i x_i \leq b\}$,
- ▶ transition probability matrix T_{KNAPSACK} has the following rules for transitioning from $s = (x_1, \dots, x_n)$ to $s' = (y_1, \dots, y_n)$
 1. Set $s' = s$ with probability $\frac{1}{2}$.
 2. Select i uniformly at random from $\{1, \dots, n\}$ and let

$$\bar{s} = (x_1, \dots, x_{i-1}, 1 - x_i, x_{i+1}, \dots, x_n).$$

3. If $\sum_{i=1}^n a_i \bar{s}_i \leq b$, then set $s' = \bar{s}$ otherwise $s' = s$.

Markov chain for the Knapsack problem

$\mathfrak{M}_{\text{KNAPSACK}} = (\Omega_{\text{KNAPSACK}}, T_{\text{KNAPSACK}})$ for Knapsack

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3. If $\sum_{i=1}^n a_i \bar{s}_i \leq b$, then set $s' = \bar{s}$ otherwise $s' = s$.

Property:

The transition probability matrix of $\mathfrak{M}_{\text{KNAPSACK}}$ is symmetric.

$$T_{u,v} = \frac{1}{2} \cdot \frac{1}{n} = T_{v,u} \text{ for } v \neq u.$$

Simulating a Markov chain

Consider a Markov chain $\mathfrak{M} = (\Omega, T)$.

Let $D : \Omega \rightarrow \mathbb{R}$ be a probability distribution on Ω .

Interpreting D as an element of $\mathbb{R}^{|\Omega|}$ we have that $D' = DT$ is also a probability distribution over Ω (since $\sum_{s' \in \Omega} T_{s,s'} = 1$).

Suppose we start in some state s_0 and simulate the Markov chain. Let X_t be the random variable such that

$X_t = s$ iff the current state at step t is s .

For the corresponding sequence of distributions $D[0], D[1], D[2], \dots$ over Ω we have that

- ▶ $D[0](s_0) = 1$ and $D_0(s) = 0$ for all $s \neq s_0$ and
- ▶ $D[i + 1] = D[i]T$ for all $i \geq 0$.

Markov Chains: Stationary distribution

Stationary distribution of a Markov chain $\mathfrak{M} = (\Omega, T)$ is a probability distribution $D : \Omega \rightarrow \mathbb{R}$ such that $DT = D$, that is,

$$\sum_{u \in \Omega} D_u \cdot T_{u,v} = D_v \text{ for all } v \in \Omega.$$

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Does every finite Markov chain have a stationary distribution? Yes.

Every stochastic matrix always has an eigenvalue of 1 with a left eigenvector whose entries are nonnegative.

Not true in general for Markov chains with infinite state space.

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Does every finite Markov chain have a unique stationary distribution?

No.

Example

Take $\mathfrak{M} = (\Omega, T)$ with $\Omega = \{u, v\}$ and $T_{u,u} = 1$ and $T_{v,v} = 1$.

Every probability distribution D on Ω is a stationary distribution.

Stationary distribution for the Knapsack problem

The uniform distribution U over Ω_{KNAPSACK} is a stationary distribution for $\mathfrak{M}_{\text{KNAPSACK}} = (\Omega_{\text{KNAPSACK}}, T_{\text{KNAPSACK}})$.

We have to show that $\sum_{s \in \Omega_{\text{KNAPSACK}}} U_s \cdot T_{s,v} = U_v$ for all v .

Consider $v \in \Omega_{\text{KNAPSACK}}$ and suppose v has d "neighbours" different from v . Recall that $T_{s,s'} = T_{s',s} = \frac{1}{2n}$ for $u \neq v$. We have

$$\begin{aligned}\sum_s U_s \cdot T_{s,v} &= U_v \cdot T_{v,v} + \sum_{s, s \neq v} U_s \cdot T_{s,v} \\ &= \frac{1}{N} \left(\frac{1}{2} + \frac{1}{2} \left(1 - \frac{d}{n} \right) \right) + d \frac{1}{N} \frac{1}{2n} \\ &= \frac{1}{N} = U_v\end{aligned}$$

Irreducible Markov chains

A **path** in $\mathfrak{M} = (\Omega, T)$ is a sequence of states $s_0, s_1 \dots s_l$ such that $T_{s_i, s_{i+1}} > 0$ for $0 \leq i < l$. We say that s_l is **reachable** from s_0 .

In the Markov chain $\mathfrak{M}_{\text{KNAPSACK}}$

- ▶ if we start from $(0, \dots, 0)$ we can reach any state,
- ▶ if we start from any state we can reach $(0, \dots, 0)$.

Thus, from any state of $\mathfrak{M}_{\text{KNAPSACK}}$ we can reach any state. Such Markov chains are called **irreducible**.

Recall the example with no unique stationary distribution.

What about convergence?

If a Markov chain has a unique stationary distribution D , does it always converge to D , starting from any distribution?

That is, for any $D[0]$, does the sequence $D[0], D[1], D[2], \dots$, where $D[i+1] = D[i]T$, converge to D ?

Not necessarily.

Example

Take $\mathfrak{M} = (\Omega, T)$ with $\Omega = \{u, v\}$ and $T_{u,v} = 1$ and $T_{v,u} = 1$.

The only stationary distribution is $D(u) = D(v) = \frac{1}{2}$.

Now, take $D[0]$ such that $D[0](u) = 1$ and $D[0](v) = 0$.

The reason for which the Markov chain does not converge is that the state **periodically** alternates between states u and v .

Aperiodic Markov chains

A state s of a Markov chain is called **periodic** if there exists $k \in \mathbb{N}$, $k > 1$ such that for every path $s = s_0, \dots, s_l = s$, k divides l .

A state which is not periodic is called aperiodic. A Markov chain is called **aperiodic** if all of its states are aperiodic.

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Is $\mathfrak{M}_{\text{KNAPSACK}}$ aperiodic? Yes.

For every state $s \in \Omega_{\text{KNAPSACK}}$, $T_{s,s} > 0$. Thus there exists a path from s to s of arbitrary length, and thus every state is aperiodic.

Fundamental Theorem of Markov chains

Theorem Every finite Markov chain \mathfrak{M} which is irreducible has a **unique stationary distribution** D , and if \mathfrak{M} is aperiodic, then it also holds that $\lim_{i \rightarrow \infty} D[i] = D$.

This means that the Markov chain $\mathfrak{M}_{\text{KNAPSACK}}$ converges to the uniform distribution over Ω_{KNAPSACK} .

Using $\mathfrak{M}_{\text{KNAPSACK}}$

Almost uniform sampling for Knapsack using $\mathfrak{M}_{\text{KNAPSACK}}$.

1. Start in state $s = (0, \dots, 0)$.
2. Simulate $\mathfrak{M}_{\text{KNAPSACK}}$ for sufficiently many steps until the distribution over states is "close" to the uniform distribution over Ω_{KNAPSACK} .
3. Return the current state.

Repeating this we can obtain a sequence of independent samples. Uniform sampling from Ω_{KNAPSACK} can be used to obtain a randomized approximation algorithm for the counting the number of solutions to the Knapsack problem.

How many steps is sufficiently many?

It is not known if $\mathfrak{M}_{\text{KNAPSACK}}$ converges to the uniform distribution in polynomial number of steps. (Ω may be exponential in n .)

Markov chain Monte Carlo

Markov chain Monte Carlo (MCMC) is a technique for sampling from a complicated distribution using local information.

The main challenge is to obtain good bounds on the number of steps a Markov chain takes to converge to the desired distribution.

MCMC may provide efficient (i.e., polynomial time) solution techniques.

Computing the volume of a convex body

Given a convex body $K \subseteq \mathbb{R}^n$, compute its volume $Vol(K)$.

The computational effort required increases as n increases.

[Dyer and Frieze'88] Computing the volume exactly is $\#\mathbf{P}$ -hard.

[Dyer, Frieze and Kannan'91] Polynomial randomized approximation algorithm via Markov chain Monte Carlo.

Input to the algorithm

K is given as a membership oracle.

Two n -dimensional balls $B_0 \subseteq K \subseteq B_r$ of non-zero radius.

By simple transformations of K it can be ensured that B_0 is the unit ball and that B_r has radius $cn \log n$ for some constant c .

Note: The volume of the smallest ball containing K might be exponential in $\text{Vol}(K)$, hence naive Monte Carlo is hopeless.

From volume computation to uniform sampling

Construct a sequence of concentric balls

$$B_0 \subseteq B_1 \subseteq \dots \subseteq K \subseteq B_r.$$

$$\text{Vol}(K) = \frac{\text{Vol}(K \cap B_r)}{\text{Vol}(K \cap B_{r-1})} \cdot \frac{\text{Vol}(K \cap B_{r-1})}{\text{Vol}(K \cap B_{r-2})} \cdot \dots \cdot \frac{\text{Vol}(K \cap B_1)}{\text{Vol}(K \cap B_0)} \cdot \text{Vol}(K \cap B_0)$$

$\text{Vol}(K \cap B_0) = \text{Vol}(B_0)$ known.

Estimate each ratio $\frac{\text{Vol}(K \cap B_i)}{\text{Vol}(K \cap B_{i-1})}$.

Sample uniformly at random from $K \cap B_i$ using MCMC and count the proportion of samples falling into B_{i-1} .

To ensure that the number of samples needed is small, ensure that the ratio $\frac{\text{Vol}(K \cap B_i)}{\text{Vol}(K \cap B_{i-1})}$ is small by making the balls grow slowly.

This implies $r = cn \log n$ for some constant c .

Time complexity

The original algorithm has time complexity $O(n^{23})$.

Later it was improved to $O(n^4)$.

Key ingredient: sample uniformly at random from the points in a convex body in **polynomial time**. For this, the Markov chain has to converge in polynomial time to the uniform distribution.

The random walk on cubes

1. Divide the space into n -dimensional (hyper)cubes of side δ .
Choose δ such to provide a good approximation of K , while permitting the random walk on the Markov chain to converge to the stationary distribution in reasonable time.
2. Perform a random walk as follows. If C is the cube at time t , select uniformly at random an orthogonally adjacent cube C' . If C' is in K , then move to C' , otherwise stay at C .

Properties:

- ▶ The uniform distribution is the unique stationary distribution.
- ▶ **Rapid mixing:** The Markov chain converges to the stationary distribution in number of steps polynomial in n .

A ball walk

Lovász and Simonovits proposed a walk with continuous space.

1. Pick $\delta \in \mathbb{R}$ by the same criteria as before.
2. Perform a random walk as follows.

If at time t the walk is at $x \in \mathbb{R}^n$, the probability density function at time $t+1$ is uniform over $K \cap B(x, \delta)$ and 0 outside.

Properties:

- ▶ Rapid mixing argument similar to the walk on cubes.
- ▶ Saves a factor n in the number of oracle calls.
- ▶ Moves more complex, so no saving in time complexity.

Conclusion

Theorem

If we can sample almost uniformly at random from Ω_{KNAPSACK} in polynomial time, then there is a polynomial-time randomized approximation scheme for the knapsack counting problem.

Theorem

There exists a polynomial time randomized approximation scheme for the volume computation problem.

Summary of today's lecture

- ▶ **Randomized algorithms:**
Power of randomness in computation, complexity classes **RP** and **BPP**, error reduction
- ▶ **Monte Carlo methods:**
Estimating the probability of a random event,
model counting via random sampling
- ▶ **Markov chain Monte Carlo methods:**
Markov chains and random walks, sampling via MCMC,
model counting via MCMC

Agenda

- Tuesday** computational complexity, probability theory
- Wednesday** randomized algorithms, Monte Carlo methods
- Thursday** hashing-based approach to model counting
- Friday** from discrete to continuous model counting