CPSC 540: Machine Learning

Topic Models

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Last Time: Empirical Bayes and Hierarchical Bayes

- In Bayesian statistics we work with posterior over parameters,

$$p(\theta \mid x, \alpha, \beta) = \frac{p(x \mid \theta)p(\theta \mid \alpha, \beta)}{p(x \mid \alpha, \beta)}.$$

- We discussed empirical Bayes, where you optimize prior using marginal likelihood,

$$\underset{\alpha,\beta}{\text{argmax}}\, p(x \mid \alpha, \beta) = \underset{\alpha,\beta}{\text{argmax}} \int_\theta p(x \mid \theta)p(\theta \mid \alpha, \beta)d\theta.$$

  - Can be used to optimize λ_j, polynomial degree, RBF σ_i, polynomial vs. RBF, etc.
- We also considered hierarchical Bayes, where you put a prior on the prior,

$$p(\alpha, \beta \mid x, \gamma) = \frac{p(x \mid \alpha, \beta)p(\alpha, \beta \mid \gamma)}{p(x \mid \gamma)}.$$

  - But is the hyper-prior really needed?

Hierarchical Bayes as a Graphical Model

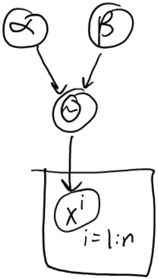
- Let x^i be a binary variable, representing if treatment works on patient i,

$$x^i \sim \text{Ber}(\theta).$$

- As before, let's assume that θ comes from a beta distribution,

$$\theta \sim \mathcal{B}(\alpha, \beta).$$

- We can visualize this as a graphical model:

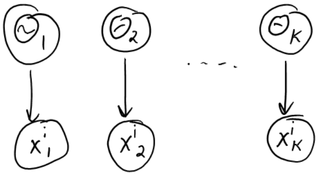


Hierarchical Bayes for Non-IID Data

- Now let x^i represent if treatment works on patient i in hospital j.
- Let's assume that treatment depends on hospital,

$$x_j^i \sim \text{Ber}(\theta_j).$$

- So the x_j^i are only IID given the hospital.



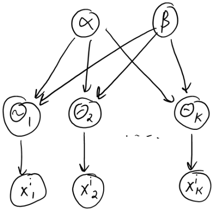
- Problem: we may not have a lot of data for each hospital.
  - Can we use data from one hospital to learn about others?
  - Can we say anything about a hospital with no data?

Hierarchical Bayes for Non-IID Data

- Common approach: assume θ_j drawn from common prior,

$$\theta_j \sim \mathcal{B}(\alpha, \beta).$$

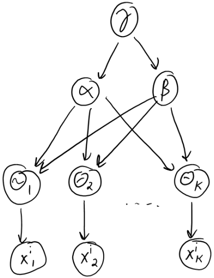
- This introduces dependency between parameters at different hospitals:



- But, if you fix α and β then you can't learn across hospitals:
  - The θ_j and d-separated given α and β.

Hierarchical Bayes for Non-IID Data

- Consider treating α and β as random variables and using a hyperprior:



- Now there is a dependency between the different θ_j.
  - Due to unknown α and β.

- Now you can combine the non-IID data across different hospitals.
  - Data-rich hospitals inform posterior for data-poor hospitals.
  - You even consider the posterior for new hospitals with no data.

Outline

Motivation for Topic Models

We want a model of the "factors" making up a set of documents.

- In this context, latent-factor models are called topic models.

Suppose you have the following set of sentences:

- I like to eat broccoli and bananas.
- I ate a banana and spinach smoothie for breakfast.
- Chinchillas and kittens are cute.
- My sister adopted a kitten yesterday.
- Look at this cute hamster munching on a piece of broccoli.

What is latent Dirichlet allocation? It's a way of automatically discovering **topics** that these sentences contain. For example, given these sentences and asked for 2 topics, LDA might produce something like

- **Sentences 1 and 2**: 100% Topic A
- **Sentences 3 and 4**: 100% Topic B
- **Sentence 5**: 60% Topic A, 40% Topic B
- **Topic A**: 30% broccoli, 15% bananas, 10% breakfast, 10% munching, ... (at which point, you could interpret topic A to be about food)
- **Topic B**: 20% chinchillas, 20% kittens, 20% cute, 15% hamster, ... (at which point, you could interpret topic B to be about cute animals)

http://blog.echen.me/2011/08/22/introduction-to-latent-dirichlet-allocation

- "Topics" could be useful for things like searching for relevant documents.

Classic Approach: Latent Semantic Indexing

- Classic methods are based on scores like TF-IDF:
  1. Term frequency: probability of a word occuring within a document.
     - E.g., 7% of words in document i are "the" and 2% of the words are "LeBron".
  2. Document frequency: probability of a word occuring across documents.
     - E.g., 100% of documents contain "the" and 0.01% have "LeBron".
  3. TF-IDF: measures like (term frequency)*log 1/(document frequency).
     - Seeing "LeBron" tells you a lot about document, seeing 'the" tells you nothing.
- Many many many variations exist.
- TF-IDF features are very redundant.
  - Consider TF-IDF of "LeBron", "Durant", and "Kobe".
  - High values of these typically just indicate topic of "basketball".
  - Basically a weighted bag of words.
- We want to find latent factors ("topics") like "basketball".

Modern Approach: Latent Dirichlet Allocation

- Latent semantic indexing (LSI) topic model:
  1. Summarize each document by its TF-IDF values.
  2. Run a latent-factor model like PCA or NMF on the matrix.
  3. Treat the latent factors as the "topics".

- LSI has largely been replace by latent Dirichlet allocation (LDA).
  - Hierarchical Bayesian model of all words in a document.
    - Still ignores word order.
    - Tries to explain all words in terms of topics.

- The most cited ML paper from the last 15 years?

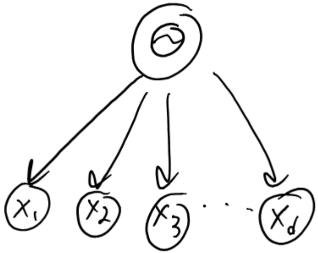
- LDA has several components, we'll build up to it by parts.
  - We'll assume all documents have d words and word order doesn't matter.

Model 1: Categorical Distribution of Words

- Base model: each word x_j comes from a categorical distribution.

$$p(x_j = \text{“the”}) = \theta_{\text{“the”}} \quad \text{where} \quad \theta_{\text{word}} \geq 0 \quad \text{and} \quad \sum_{\text{word}} \theta_{\text{word}} = 1.$$

- So to generate a document with d words:
  - Sample d words from the categorical distribution.

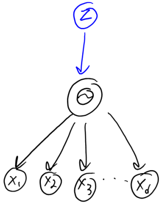


- Drawback: misses that dcouments are about different “topics”.
  - We want the word distribution to depend on the “topics”.

Model 2: Mixture of Categorical Distributions

- To represent "topics", we'll use a mixture model.
  - Each mixture has its own categorical distribution over words.
    - E.g., the "basketball" mixture will have higher probability of "LeBron".

- So to generate a document with d words:
  - Sample a topic z from a categorical distribution.
  - Sample d word categorical distribution z.

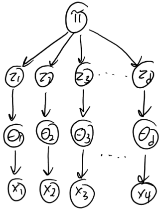


- Drawback: misses that documents may be about more than one topics.

Model 3: Multi-Topic Mixture of Categorical

- Our third model introduces a new vector of “topic proportions” π.
  - Gives percentage of each topic that makes up the document.
    - E.g., 80% basketball and 20% politics.
  - Called probabilistic latent semantic indexing (PLSI).

- So to generate a document with d words given topic proportions π:
  - Sample d topics z_j from categorical distribution π.
  - Sample a word for each z_j from corresponding categorical distribution.

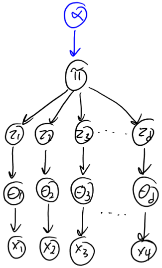


- Drawback: how do we compute π for a new document?
  - This is the same issue we had in our hospitals example.

Model 4: Latent Dirichlet Allocation

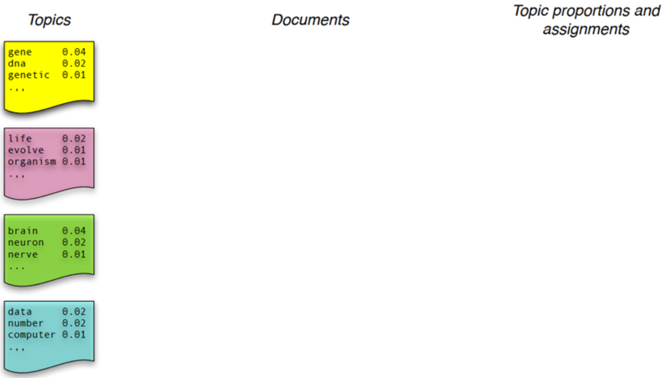
- Latent Dirichlet allocation (LDA) puts a prior on topic proportions.
  - Conjugate prior for categorical is Dirichlet distribution.

- So to generate a document with d words given Dirichlet prior:
  - Sample mixture proportions π from the Dirichlet prior.
  - Sample d topics z_j from categorical distribution π.
  - Sample a word for each z_j from corresponding categorical distribution.



- This is the generative model, typically fit with MCMC or variational methods.

Latent Dirichlet Allocation (LDA)



Each topic is like a "principal component" or "latent factor"

http://menome.com/wp/wp-content/uploads/2014/12/Blei2011.pdf

Latent Dirichlet Allocation (LDA)

1. Sample topic proportions θ from Dirichlet.

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Latent Dirichlet Allocation (LDA)

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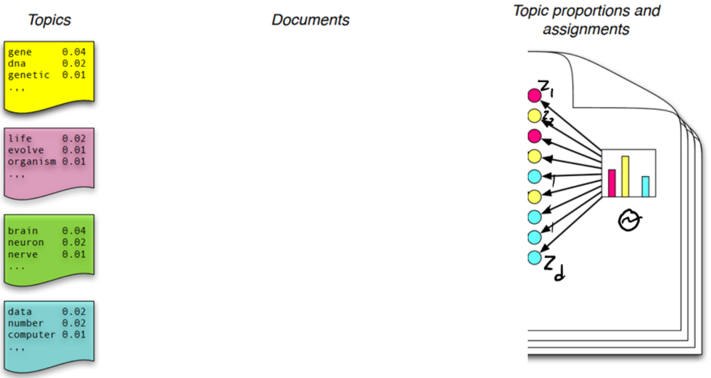

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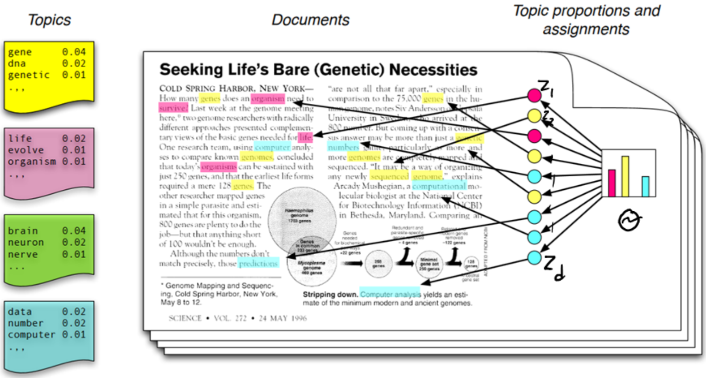
Latent Dirichlet Allocation (LDA)

1. Sample topic proportions θ from Dirichlet.

2. Sample 'd' topics z_j from θ.

3. For each z_j sample a word based on frequencies for topic.



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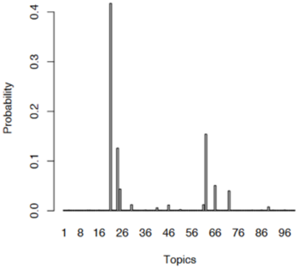
Latent Dirichlet Allocation Example



"Genetics"	**"Evolution"**	**"Disease"**	**"Computers"**
human	evolution	disease	computer
genome	evolutionary	host	models
dna	species	bacteria	information
genetic	organisms	diseases	data
genes	life	resistance	computers
sequence	origin	bacterial	system
gene	biology	new	network
molecular	groups	strains	systems
sequencing	phylogenetic	control	model
map	living	infectious	parallel
information	diversity	malaria	methods
genetics	group	parasite	networks
mapping	new	parasites	software
project	two	united	new
sequences	common	tuberculosis	simulations

Figure 2: **Real inference with LDA.** We fit a 100-topic LDA model to 17,000 articles from the journal *Science*. At left is the inferred topic proportions for the example article in Figure 1. At right are the top 15 most frequent words from the most frequent topics found in this article.

http://menome.com/wp/wp-content/uploads/2014/12/Blei2011.pdf

Latent Dirichlet Allocation Example

Figure 3: A topic model fit to the *Yale Law Journal*. Here there are twenty topics (the top eight are plotted). Each topic is illustrated with its top most frequent words. Each word's position along the x-axis denotes its specificity to the documents. For example "estate" in the first topic is more specific than "tax."

http://menome.com/wp/wp-content/uploads/2014/12/Blei2011.pdf

Latent Dirichlet Allocation Example

Health topics in social media:

Non-Ailment Topics

TV & Movies	Games & Sports	School	Conversation	Family	Transportation	Music
watch	killing	ugh	ill	mom	home	voice
watching	play	class	ok	shes	car	hear
tv	game	school	haha	dad	drive	feelin
killing	playing	read	ha	says	walk	lil
movie	win	test	fine	hes	bus	night
seen	boys	doing	yeah	sister	driving	bit
movies	games	finish	thanks	tell	trip	music
mr	fight	reading	hey	mum	ride	listening
watched	lost	teacher	thats	brother	leave	listen
hi	team	write	xd	thinks	house	sound

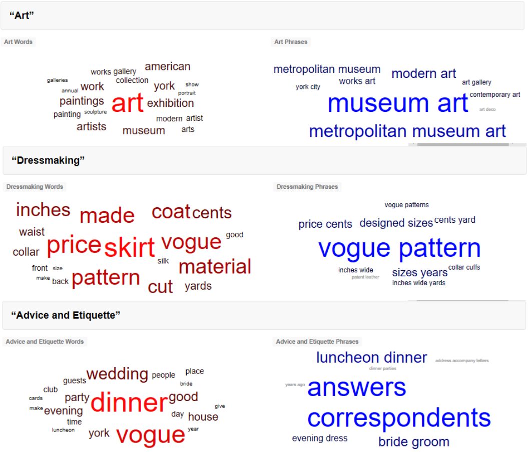
Ailments

	Influenza-like Illness	Insomnia & Sleep Issues	Diet & Exercise	Cancer & Serious Illness	Injuries & Pain	Dental Health
General Words	better	night	body	cancer	hurts	dentist
	hope	bed	pounds	help	knee	appointment
	ill	body	gym	pray	ankle	doctors
	soon	ill	weight	awareness	hurt	tooth
	feel	tired	lost	diagnosed	neck	teeth
	feeling	work	workout	prayers	ouch	appt
	day	day	lose	died	leg	wisdom
	flu	hours	days	family	arm	eye
	thanks	asleep	legs	friend	fell	going
	xx	morning	week	shes	left	went
Symptoms	sick	sleep	sore	cancer	pain	infection
	sore	headache	throat	breast	sore	pain
	throat	fall	pain	lung	head	mouth
	fever	insomnia	aching	prostate	foot	ear
	cough	sleeping	stomach	sad	feet	sinus
Treatments	hospital	sleeping	exercise	surgery	massage	surgery
	surgery	pills	diet	hospital	brace	braces
	antibiotics	caffeine	dieting	treatment	physical	antibiotics
	fluids	pill	exercises	heart	therapy	eye
	paracetamol	tylenol	protein	transplant	crutches	hospital

http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0103408

Latent Dirichlet Allocation Example

Three topics in 100 years of "Vogue" fashion magazine:



http://dh.library.yale.edu/projects/vogue/topics/

Discussion of Topic Models

- There are *many* extensions of LDA:
    - We can put prior on the number of words (like Poisson).
    - Correlated and hierarchical topic models learn dependencies between topics.

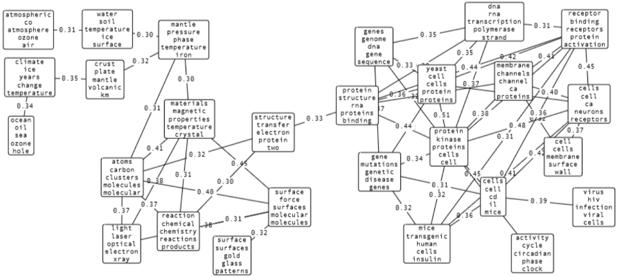


Figure 2: A portion of the topic graph learned from 15,744 OCR articles from *Science*. Each node represents a topic, and is labeled with the five most probable words from its distribution; edges are labeled with the correlation between topics.

http://people.ee.duke.edu/~lcarin/Blei2005CTM.pdf

Discussion of Topic Models

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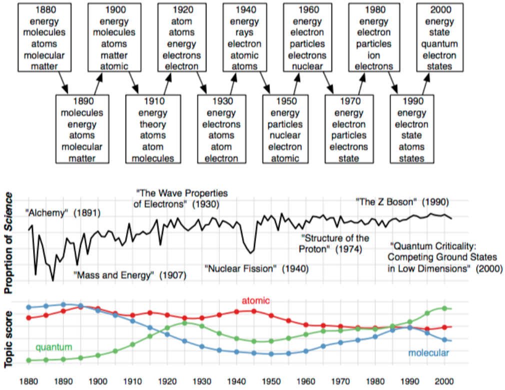
  - Can be combined with Markov models to capture dependencies over time.



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Discussion of Topic Models

- There are *many* extensions of LDA:
    - We can put prior on the number of words (like Poisson).
    - Correlated and hierarchical topic models learn dependencies between topics.
    - Can be combined with Markov models to capture dependencies over time.
    - Recent work on better word representations like "word2vec" (bonus slides).
    - Now being applied beyond text, like "cancer mutation signatures":

http://journals.plos.org/plosgenetics/article?id=10.1371/journal.pgen.1005657

Discussion of Topic Models

- Topic models for analyzing musical keys:

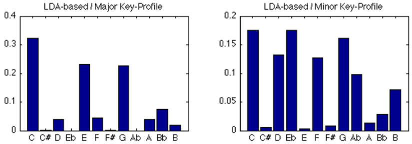


Figure 2: The C major and C minor key-profiles learned by our model, as encoded by the β matrix. Resulting key-profiles are obtained by transposition.

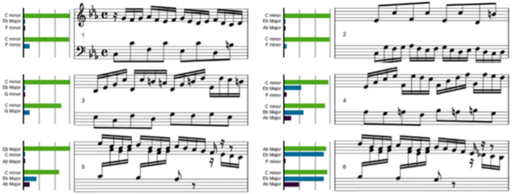


Figure 3: Key judgments for the first 6 measures of Bach's Prelude in C minor, WTC-II. Annotations for each measure show the top three keys (and relative strengths) chosen for each measure. The top set of three annotations are judgments from our LDA-based model; the bottom set of three are from human expert judgments [3].

Monte Carlo Methods for Topic Models

- Nasty integrals in topic models:

Inference [edit]

See also: Dirichlet-multinomial distribution

Learning the various distributions (the set of topics, their associated word probabilities, the topic of each word, and the particular topic mixture of each document) is a problem of Bayesian inference. The original paper used a variational Bayes approximation of the posterior distribution;[1] alternative inference techniques use Gibbs sampling[6] and expectation propagation.[7]

Following is the derivation of the equations for collapsed Gibbs sampling, which means φs and θs will be integrated out. For simplicity, in this derivation the documents are all assumed to have the same length N. The derivation is equally valid if the document lengths vary.

According to the model, the total probability of the model is:

$$P(\boldsymbol{W},\boldsymbol{Z},\boldsymbol{\theta},\boldsymbol{\varphi};\alpha,\beta)=\prod_{i=1}^{K}P(\varphi_i;\beta)\prod_{j=1}^{M}P(\theta_j;\alpha)\prod_{t=1}^{N}P(Z_{j,t}|\theta_j)P(W_{j,t}|\varphi_{Z_{j,t}}),$$

where the bold-font variables denote the vector version of the variables. First, $\boldsymbol{\varphi}$ and $\boldsymbol{\theta}$ need to be integrated out.

$$\begin{aligned}P(\boldsymbol{Z},\boldsymbol{W};\alpha,\beta)&=\int_{\boldsymbol{\theta}}\int_{\boldsymbol{\varphi}}P(\boldsymbol{W},\boldsymbol{Z},\boldsymbol{\theta},\boldsymbol{\varphi};\alpha,\beta)\,d\boldsymbol{\varphi}\,d\boldsymbol{\theta}\\&=\int_{\boldsymbol{\varphi}}\prod_{i=1}^{K}P(\varphi_i;\beta)\prod_{j=1}^{M}\prod_{t=1}^{N}P(W_{j,t}\mid\varphi_{Z_{j,t}})\,d\boldsymbol{\varphi}\int_{\boldsymbol{\theta}}\prod_{j=1}^{M}P(\theta_j;\alpha)\prod_{t=1}^{N}P(Z_{j,t}\mid\theta_j)\,d\boldsymbol{\theta}.\end{aligned}$$

https://en.wikipedia.org/wiki/Latent_Dirichlet_allocation

Monte Carlo Methods for Topic Models

- How do we actually *use* Monte Carlo for topic models?
- First we write out the posterior:

$$p(Z, \pi, \theta \mid X, \alpha, \beta) = \left[\prod_{i=1}^{n} \underbrace{p(\theta^i \mid \alpha)}_{\substack{\text{topic proportion}\\ \text{probability}\\ \text{(document 'i')}}} \prod_{j=1}^{d} \underbrace{p(z_j^i \mid \theta^i)}_{\substack{\text{topic probability}\\ \text{(topic at position}\\ \text{'j' in document 'i')}}} \underbrace{p(x_j^i \mid z_j^i, \pi_j)}_{\substack{\text{word probability}\\ \text{(word at position}\\ \text{'j' in document 'i')}}}\right]\left[\prod_{c=1}^{k} \underbrace{p(\pi_c \mid \beta)}_{\substack{\text{word probability}\\ \text{parameters}\\ \text{(topic 'c')}}}\right]$$

topics

word prob.

topic prop.

data (words)

prior on topic proportions

prior on word probabilities

Monte Carlo Methods for Topic Models

- How do we actually *use* Monte Carlo for topic models?
- Next we generate samples from the posterior:
  - With Gibbs sampling we alternate between:
    - Samplign topics given word probabilities and topic proportions.
    - Sampling topic proportions given topics and prior parameters α.
    - Sampling word probabilities given topics, words, and prior parameters β.
  - Have a burn-in period, use thinning, try to monitor convergence, etc.
- Finally, we use posterior sampeles to do inference:
  - Distribution of topic proportions for sample i is frequency in samples.
  - To see if words come from same topic, check frequency in samples.

Outline

Overview of Bayesian Inference Tasks

- In Bayesian approach, we typically work with the posterior

$$p(\theta \mid x) = \frac{1}{Z} p(x \mid \theta) p(\theta),$$

  where Z makes the distribution sum/integrate to 1.

- Typically, we need to compute expectation of some f with respect to posterior,

$$E[f(\theta)] = \int_{\theta} f(\theta) p(\theta \mid x) d\theta.$$

- Examples:
  - If $f(\theta) = \theta$, we get posterior mean of θ.
  - If $f(\theta) = p(\tilde{x} \mid \theta)$, we get posterior predictive.
  - If $f(\theta) = \mathbb{I}(\theta \in S)$ we get probability of S (e.g., marginals or conditionals).
  - If $f(\theta) = 1$ and we use $\tilde{p}(\theta \mid x)$, we get marginal likelihood Z.

Need for Approximate Integration

- Bayesian models allow things that aren't possible in other frameworks:
  - Optimize the regularizer (empirical Bayes).
  - Relax IID assumption (hierarchical Bayes).
  - Have clustering happen on multiple leves (topic models).

- But posterior often doesn't have a closed-form expression.
  - We don't just want to flip coins and multiply Gaussians.

- We once again need approximate inference:
  1. Variational methods.
  2. Monte Carlo methods.

- Classic ideas from statistical physics, that revolutionized Bayesian stats/ML.

Variational Inference vs. Monte Carlo

Two main strategies for approximate inference:

1. Variational methods:
   - Approximate p with "closest" distribution q from a tractable family,
     $$p(x) \approx q(x).$$
   - Turns inference into optimization (need to find best q).
     - Called variational Bayes.
2. Monte Carlo methods:
   - Approximate p with empirical distribution over samples,
     $$p(x) \approx \frac{1}{n}\sum_{i=1}^{n} \mathcal{I}[x^i = x].$$
   - Turns inference into sampling.
     - For Bayesian methods, we'll typically need to sample from posterior.

Conjugate Graphical Models: Ancestral and Gibbs Sampling

- For conjugate DAGs, we can use ancestral sampling for unconditional sampling.
- Examples:
  - For LDA, sample π then sample the z_j then sample the x_j.
  - For HMMs, sample the hidden z_j then sample the x_j.
- We can also often use Gibbs sampling as an approximate sampler.
  - If neighbours are conjugate in UGMs.
  - To generate conditional samples in conjugate DAGs.
- However, without conjugacy our inverse transform trick doesn't work.
  - We can't even sample from the 1D conditionals with this method.

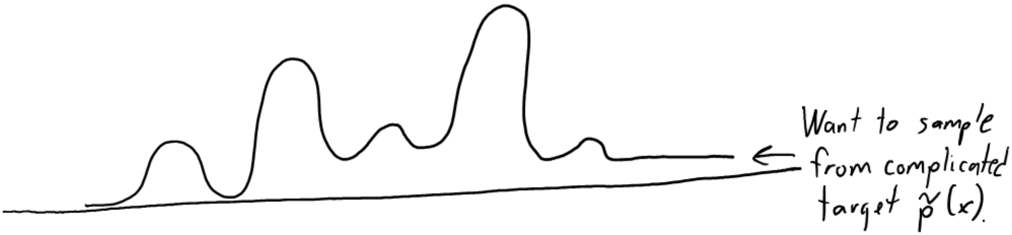
Beyond Inverse Transform and Conjugacy

- We want to use simple distributions to sample from complex distributions.
- Two common strategies are rejection sampling and importance sampling.

- We've previously seen rejection sampling to do conditional sampling:
  - Example: sampling from a Gaussian subject to $x \in [-1, 1]$.

  - Generate unconditional samples, throw out the ones that aren't in $[-1, 1]$.

General Rejection Sampling Algorithm



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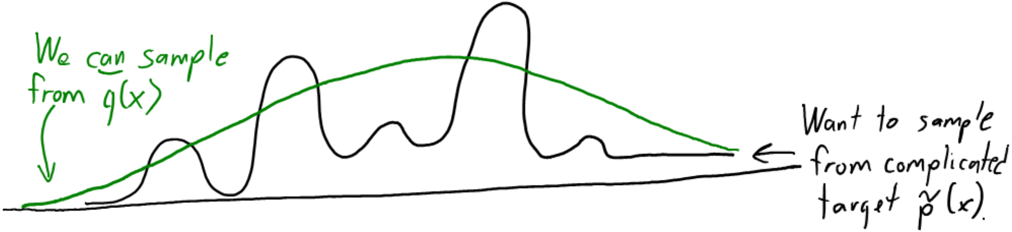

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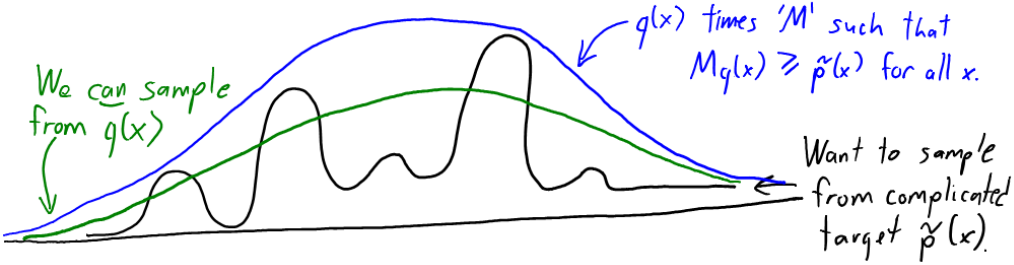

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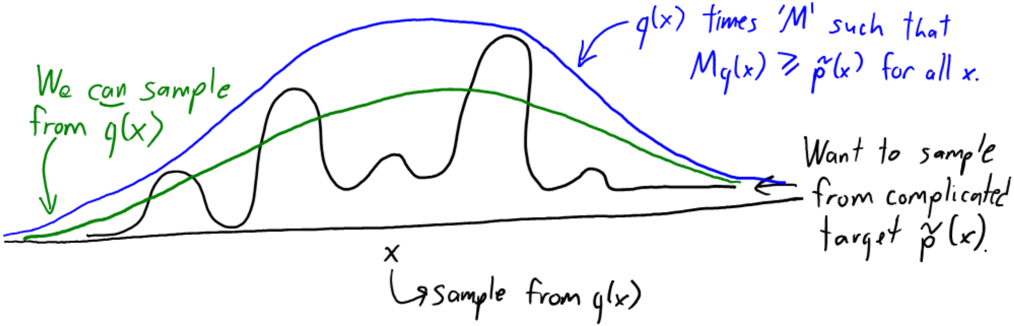

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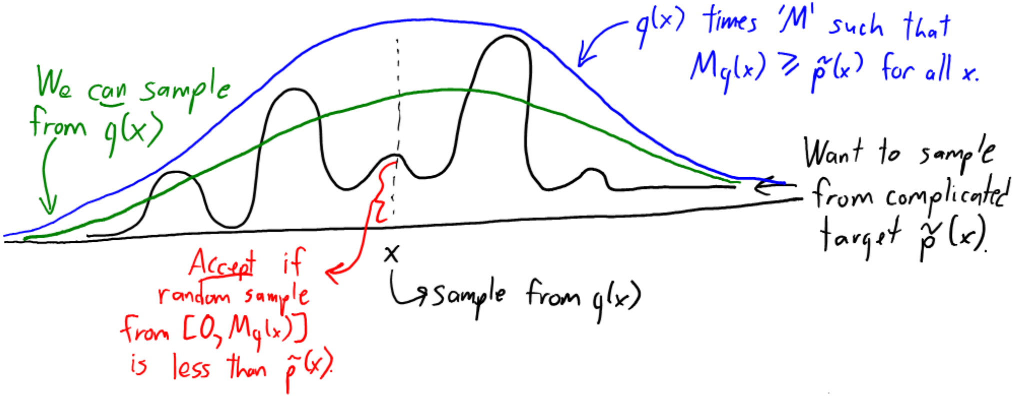

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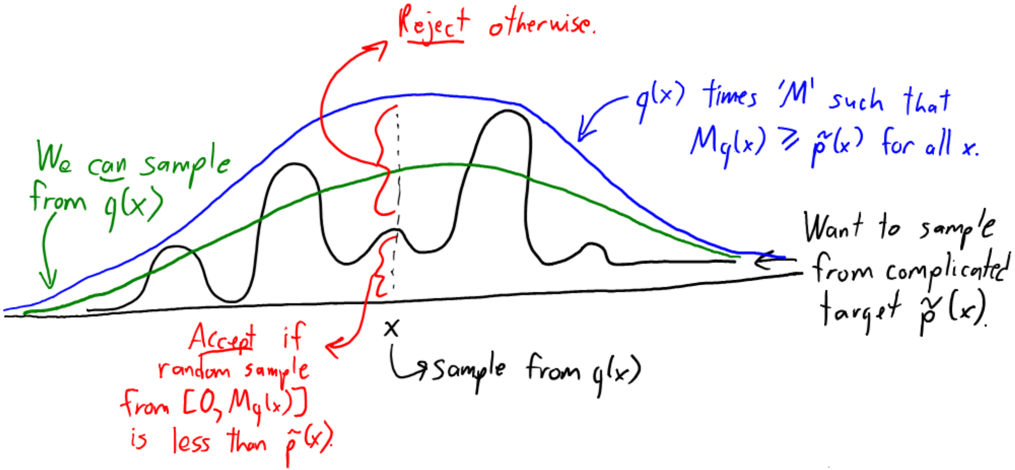
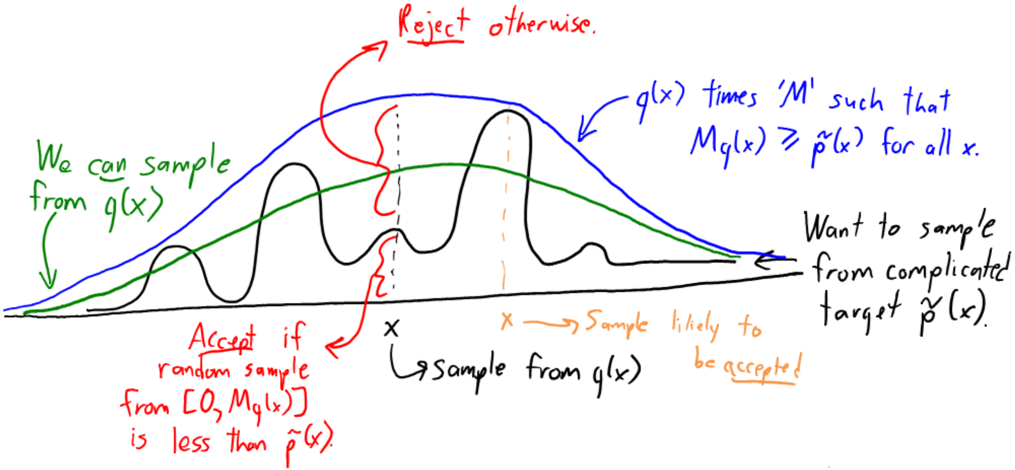
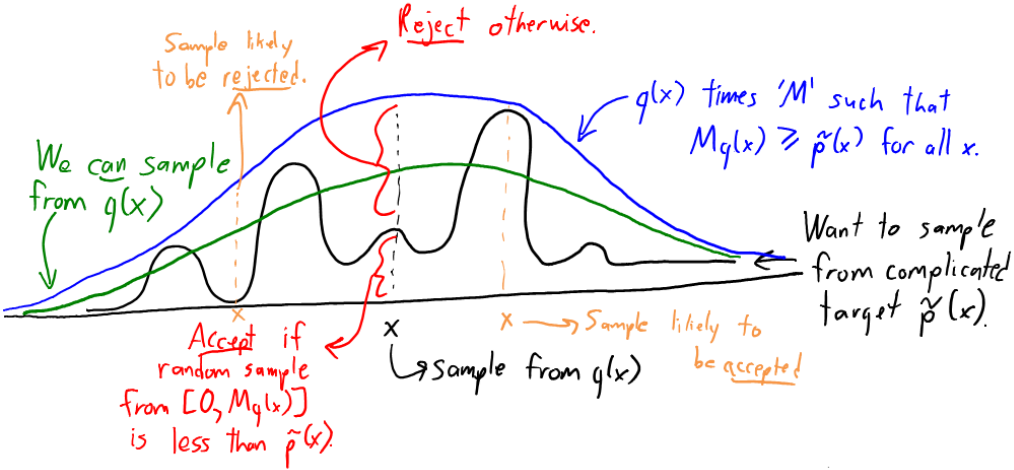


General Rejection Sampling Algorithm



General Rejection Sampling Algorithm



General Rejection Sampling Algorithm

- Ingredients of a more general rejection sampling algorithm:
  1. Ability to evaluate unnormalized $\tilde{p}(x)$,
  $$p(x) = \frac{\tilde{p}(x)}{Z}.$$
  2. A distribution q that is easy to sample from.
  3. An upper bound M on $\tilde{p}(x)/q(x)$.

- Rejection sampling algorithm:
  1. Sample x from $q(x)$.
  2. Sample u from $\mathcal{U}(0,1)$.
  3. Keep the sample if $u \leq \frac{\tilde{p}(x)}{Mq(x)}$.
- The accepted samples will be from $p(x)$.

General Rejection Sampling Algorithm

- We can use general rejection sampling for:
  - Sample from Gaussian q to sample from student t.
  - Sample from prior to sample from posterior $(M = 1)$,

$$p(\theta \mid x) = \underbrace{p(x \mid \theta)}_{\leq 1} p(\theta).$$

- Drawbacks:
  - You may reject a large number of samples.
    - Most samples are rejected for high-dimensional complex distributions.
  - You need to know M.

- Extension in 1D for convex $-\log p(x)$:
  - Adaptive rejection sampling refines piecewise-linear q after each rejection.

Importance Sampling

- Importance sampling is a variation that accepts all samples.
  - Key idea is similar to EM,

$$\begin{aligned}\mathbb{E}_p[f(x)] &= \sum_x p(x)f(x)\\ &= \sum_x q(x)\frac{p(x)f(x)}{q(x)}\\ &= \mathbb{E}_q\left[\frac{p(x)}{q(x)}f(x)\right],\end{aligned}$$

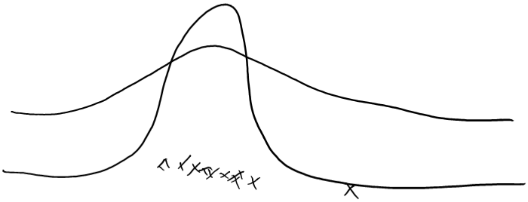
  and similarly for continuous distributions.

  - We can sample from q but reweight by $p(x)/q(x)$ to sample from p.
  - Only assumption is that q is non-zero when p is non-zero.
  - If you only know unnormalized $\tilde{p}(x)$, a variant gives approximation of Z.

Importance Sampling

- As with rejection sampling, only efficient if q is close to p.
- Otherwise, weights will be huge for a small number of samples.
  - Even though unbiased, variance will be huge.

- Can be problematic if q has lighter "tails" than p:
  - You rarely sample the tails, so those samples get huge weights.



- As with rejection sampling, doesn't tend to work well in high dimensions.

Outline

Limitations of Simple Monte Carlo Methods

- The basic ingredients of our previous sampling methods:
  - Inverse CDF, rejection sampling, importance sampling.
  - Sampling in higher-dimensions: ancestral sampling, Gibbs sampling.
- These work well in low dimensions or for posteriors with analytic properties.
- But we want to solve high-dimensional integration problems in other settings:
  - Deep belief networks and Boltzmann machines.
  - Bayesian graphical models and Bayesian neural networks.
  - Hierarchical Bayesian models.
- Our previous methods tend not to work in complex situations:
  - Inverse CDF may not be available.
  - Conditionals needed for ancestral/Gibbs sampling may be hard to compute.
  - Rejection sampling tends to reject almost all samples.
  - Importance sampling tends to give almost zero weight to all samples.

Dependent-Sample Monte Carlo Methods

- We want an algorithm whose samples get better over time.
- Two main strategies for generating dependent samples:
  - Sequential Monte Carlo:
    - Importance sampling where proposal q_t changes over time from simple to posterior.
    - "Particle Filter Explained without Equations": `https://www.youtube.com/watch?v=aUkBa1zMKv4`
    - AKA sequential importance sampling, annealed importance sampling, particle filter.
  - Markov chain Monte Carlo (MCMC).
    - Design Markov chain whose stationary distribution is the posterior.
- These are the main tools to sample from high-dimensional distributions.

Markov Chain Monte Carlo

- We've previously discussed Markov chain Monte Carlo (MCMC).
  1. Based on generating samples from a Markov chain q.
  2. Designed so stationary distribution π of q is target distribution p.

- If we run the chain long enough, it gives us samples from p.

- Gibbs sampling is an example of an MCMC method.
  - Sample x_j conditioned on all other variables x_{-j}.

- Note that before we were sampling states according to a UGM, now we're sampling parameters according to the posterior.

Limitations of Gibbs Sampling

- Gibbs sampling is nice because it has no parameters:
  - You just need to decide on the blocks and figure out the conditionals.
- But it isn't always ideal:
  - Samples can be very correlated: slow progress.
  - Conditionals may not have a nice form:
    - If Markov blanket is not conjugate, need rejection/importance sampling.
- Generalization that can address these is Metropolis-Hastings:
  - Oldest algorithm among the "10 Best of the 20th Century".

Warm-Up to Metropolis-Hastings: "Stupid MCMC"

- Consider finding the expected value of a fair di:
  - For a 6-sided di, the expected value is 3.5.
- Consider the following "stupid MCMC" algorithm:
  - Start with some initial value, like "4".
  - At each step, roll the di and generate a random number u:
    - If $u < 0.5$, "accept" the roll and take the roll as the next sample.
    - Othewise, "rejeect" the roll and take the old value ("4") as the next sample.

Warm-Up to Metropolis-Hastings: "Stupid MCMC"

- Example:
  - Start with "4", so record "4".
  - Roll a 6 and generate 0.234, so record 6.
  - Roll a 3 and generate 0.612, so record 6.
  - Roll a 2 and generate 0.523, so record 6.
  - Roll a 3 and generate 0.125, so record 3.
- So our samples are 4,6,6,6,3,...
  - If you run this long enough, you will spend 1/6 of the time on each number.
  - So the dependent samples from this Markov chain could be used within Monte Carlo.
- Its stupid since you should just accept every sample (theyre IID samples).
  - It works but its twice as slow.

A Simple Example of Metropolis-Hastings

- Consider a loaded di that rolls a 6 half the time.
  - All others are equally likely, so they have probability $1/10$.

- Consider the following "less stupid" MCMC algorithm:
  - At each step, we start with an old state x.
  - Generate a random number x uniformly between 1 and 6 (roll a fair di), and generate a random number u in the interval $[0, 1]$.
  - "Accept" this roll if

$$u < \frac{p(\hat{x})}{p(x)}.$$

  - So if we roll $\hat{x} = 6$, we accept it: $u < 1$ ("always move to higher probability").
  - If $x = 2$ and roll $\hat{x} = 1$, accept it: $u < 1$ ("always move to same probability").
  - If $x = 6$ and roll $\hat{x} = 1$, we accept it with probability $1/5$.
    - We prefer high probability states, but sometimes move to low probability states.

- This has right probabilities as the stationary distribution (not yet obvious).
  - And accepts most samples.

Metropolis Algorithm

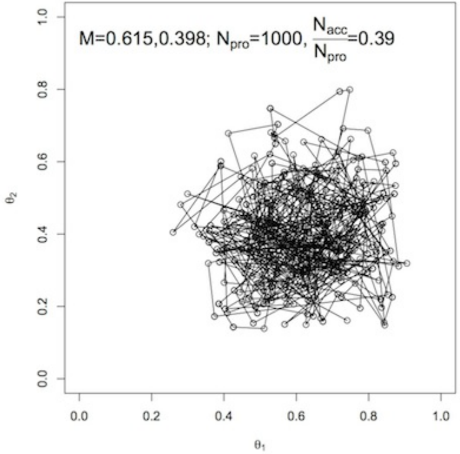
- The Metropolis algorithm for sampling from a continuous target $p(x)$:
  - On each iteration add zero-mean Gaussian noise to x^t to give proposal $\hat{x}^t$.
  - Generate u uniformly between 0 and 1.
  - "Accept" the sample and set $x^{t+1} = \hat{x}^t$ if

$$u \leq \frac{\tilde{p}(\hat{x}^t)}{\tilde{p}(x^t)}, \qquad \frac{\text{(probability of proposed)}}{\text{(probability of current)}}$$

  - Otherwise "reject" the sample and use x^t again as the next sample x^{t+1}.

- A random walk, but sometimes rejecting steps that decrease probability:
  - A valid MCMC algorithm on continuous densities, but convergence may be slow.
  - You can implement this even if you don't know normalizing constant.

Metropolis Algorithm in Action



Pseudo-code:

```
eps = randn(d,1)
xhat = x + eps
u = rand()
if u < ( p(xhat) / p(x) )
 set x = xhat
otherwise
  keep x
```

Metropolis Algorithm Analysis

- Markov chain with transitions $q_{ss'} = q(x^t = s' \mid x^{t-1} = s)$ is reversible if

$$\pi(s)q_{ss'} = \pi(s')q_{s's},$$

for some distribution π (this condition is called detailed balance).

- Assuming we reach stationary, reversibility implies π is stationary distribution.
    - By summing reversibility condition over all s values we get

$$\sum_s \pi(s)q_{ss'} = \sum_s \pi(s')q_{s's}$$

$$\sum_s \pi(s)q_{ss'} = \pi(s')\underbrace{\sum_s q_{s's}}_{=1}$$

$$\sum_s \pi(s)q_{ss'} = \pi(s') \qquad \text{(stationary condition).}$$

- Metropolis is reversible (bonus slide) so has correct stationary distribution.

Metropolis-Hastings

- Gibbs and Metropolis are special cases of Metropolis-Hastings.
  - Uses a proposal distribution $q(\hat{x} \mid x)$, giving probability of proposing $\hat{x}$ at x.
    - In Metropolis, q is a zero-mean Gaussian.

- Metropolis-Hastings accepts a proposed $\hat{x}^t$ if

$$u \leq \frac{\tilde{p}(\hat{x}^t)q(x^t \mid \hat{x}^t)}{\tilde{p}(x^t)q(\hat{x}^t \mid x^t)},$$

where extra terms ensure reversibility for asymmetric q:

  - E.g., if you are more likely to propose to go from x^t to $\hat{x}^t$ than the reverse.

- This again works under very weak conditions, such as $q(\hat{x}^t \mid x^t) > 0$.
  - You can make performance much better/worse with an appropriate q.

Metropolis-Hastings Example: Rolling Dice with Coins

- Conisder the following random walk on the numbers 1-6:
  - If $x = 1$, always propose 2.
  - If $x = 2$, 50% of the time propose 1 and 50% of the time propose 3.
  - If $x = 3$, 50% of the time propose 2 and 50% of the time propose 4.
  - If $x = 4$, 50% of the time propose 3 and 50% of the time propose 5.
  - If $x = 5$, 50% of the time propose 4 and 50% of the time propose 6.
  - If $x = 6$, always propose 5.

- "Flip a coin: go up if it's heads and go down it it's tails".
  - The PageRank "random surfer" applied to this graph:

Metropolis-Hastings Example: Rolling Dice with Coins

- Suppose we want to sample for a fair 6-sided di.
  - p(x=1) = p(x=2) = p(x=3) = p(x=4) = p(x=5) = p(x=6) = 1/6.
  - But don't have a di or a computer and can only flip coins.

- Use random walk as transitions q in Metropolis-Hastings.
  - $q(\hat{x} = 2 \mid x = 1) = 1$, $q(\hat{x} = 1 \mid x = 2) = \frac{1}{2}$, $q(\hat{x} = 2 \mid x = 3) = 1/2, \ldots$
  - If x is in the "middle" (2-5), we'll always accept the random walk.
    - If $x = 3$ and we propose $\hat{x} = 2$, then:

$$u < \frac{p(\hat{x} = 2)}{p(x = 3)} \frac{q(x = 3 \mid \hat{x} = 2)}{q(\hat{x} = 2 \mid x = 3)} = \frac{1/6}{1/6} \frac{1/2}{1/2} = 1.$$

    - If $x = 2$ and we propose $\hat{x} = 1$, then we test $u < 2$ which is also always true.

    - If x is at the end $(1$ or $6)$, you accept with probability $1/2$:

$$u < \frac{p(\hat{x} = 2)}{p(x = 1)} \frac{q(x = 1 \mid \hat{x} = 2)}{q(\hat{x} = 2 \mid x = 1)} = \frac{1/6}{1/6} \frac{1/2}{1} = \frac{1}{2}.$$

Metropolis-Hastings Example: Rolling Dice with Coins

- So Metropolis-Hastings modifies random walk probabilities:
  - If you're at the end (1 or 6), stay there half the time.
  - This accounts for the fact that 1 and 6 have only one neighbour.
    - Which means they aren't visited as often by the random walk.

- Could also be viewed as a random surfer in a different graph:

- You can think of Metropolis-Hastings as the modification that "makes the random walk have the right probabilities".
  - For any (reasonable) proposal distribution q.

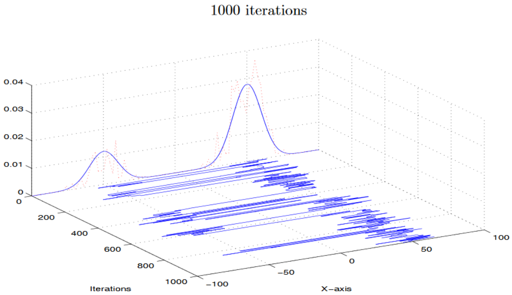
Metropolis-Hastings

- Simple choices for proposal distribution q:
  - Metropolis originally used random walks: $x^t = x^{t-1} + \epsilon$ for $\epsilon \sim \mathcal{N}(0, \Sigma)$.
  - Hastings originally used independent proposal: $q(x^t \mid x^{t-1}) = q(x^t)$.
  - Gibbs sampling updates single variable based on conditional:
    - In this case the acceptance rate is 1 so we never reject.
  - Mixture model for q: e.g., between big and small moves.
  - "Adaptive MCMC": tries to update q as we go: needs to be done carefully.
  - "Particle MCMC": use particle filter to make proposal.

- Unlike rejection sampling, we don't want acceptance rate as high as possible:
  - High acceptance rate may mean we're not moving very much.
  - Low acceptance rate definitely means we're not moving very much.
  - Designing q is an "art".

Mixture Proposal Distribution

Metropolis-Hastings for sampling from mixture of Gaussians:



http://www.cs.ubc.ca/~arnaud/stat535/slides10.pdf

- With a random walk q we may get stuck in one mode.
- We could have proposal be mixture between random walk and "mode jumping".

Advanced Monte Carlo Methods

- Some other more-powerful MCMC methods:
  - Block Gibbs sampling improves over single-variable Gibb sampling.
  - Collapsed Gibbs sampling (Rao-Blackwellization): integrate out variables that are not of interest.
    - E.g., integrate out hidden states in Bayesian hidden Markov model.
    - E.g., integrate over different components in topic models.
    - Provably decreases variance of sampler (if you can do it, you should do it).
  - Auxiliary-variable sampling: introduce variables to sample bigger blocks:
    - E.g., introduce z variables in mixture models.
    - Also used in Bayesian logistic regression (beginning with Albert and Chib).

Advanced Monte Carlo Methods

- Trans-dimensional MCMC:
  - Needed when dimensionality of problem can change on different iterations.
  - Most important application is probably Bayesian feature selection.

- Hamiltonian Monte Carlo:
  - Faster-converging method based on Hamiltonian dynamics.
  - I think Alex will discuss this next time.

- Population MCMC:
  - Run multiple MCMC methods, each having different "move" size.
  - Large moves do exploration and small moves refine good estimates.

- Combinations of variational inference and stochastic methods:
  - Variational MCMC: Metropolis-Hastings where variational q can make proposals.
  - Stochastic variational inference (SVI): variational methods using stochastic gradient.

Summary

- Relaxing IID assumption with hierarchical Bayes.
- Latent Dirichlet allocation: factor/topic model for discrete data like text.
- Rejection sampling: generate exact samples from complicated distributions.
- Importance sampling: reweights samples from the wrong distribution.
- Markov chain Monte Carlo generates a sequence of *dependent samples*:
  - But asymptotically these samples come from the posterior.
- Metropolis-Hastings allows arbitrary "proposals".
  - With good proposals works much better than Gibbs sampling.

- Guest lecture by Alex Bouchard, then next week npBayes/variational/VAE/GANs.

Metropolis Algorithm Analysis

- Metropolis algorithm has $q_{ss'} > 0$ (sufficient to guarantee stationary distribution is unique and we reach it) and satisfies detailed balance with target distribution p,
$$p(s)q_{ss'} = p(s')q_{s's}.$$
- We can show this by defining transition probabilities
$$q_{ss'} = \min\left\{1, \frac{\tilde{p}(s')}{\tilde{p}(s)}\right\},$$
and observing that
$$\begin{aligned}
p(s)q_{ss'} &= p(s)\min\left\{1, \frac{\tilde{p}(s')}{\tilde{p}(s)}\right\} = p(s)\min\left\{1, \frac{\frac{1}{Z}\tilde{p}(s')}{\frac{1}{Z}\tilde{p}(s)}\right\} \\
&= p(s)\min\left\{1, \frac{p(s')}{p(s)}\right\} = \min\left\{p(s), p(s')\right\} \\
&= p(s')\min\left\{1, \frac{p(s)}{p(s')}\right\} = p(s')q_{s's}.
\end{aligned}$$

Latent-Factor Representation of Words

- In natural language, we often represent words by an index.
  - E.g., "cat" is word 124056 among a "bag of words".
- But this may be innefficient:
  - Should "cat" and "kitten" share parameters in some way?
- We want a latent-factor representation of words.
  - Closeness in latent space should indicate similarity.
  - Distances could represent meaning?
- We could use PCA, LDA, and so on.
- But recent "word2vec" approach is getting a lot of popularity...

Using Context

- Consider these phrases:
  - "The *cat* purred".
  - "The *kitten* purred".

  - "black *cat* ran".
  - "black *kitten* ran"
- Words that occur in the same context likely have similar meanings.
- Word2vec uses this insight to design an MDS distance function.

Word2Vec

- Two variations of word2vec:
  1. Try to predict word from surrounding words ("continuous bag of words").
  2. Try to predict surrounding words from word ("skip-gram").

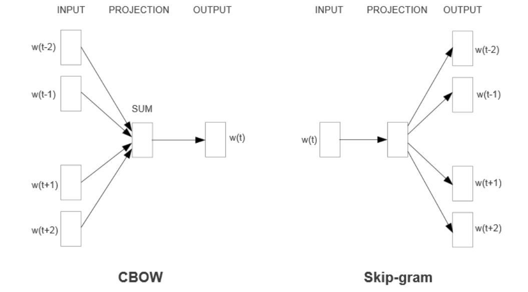


Figure 1: New model architectures. The CBOW architecture predicts the current word based on the context, and the Skip-gram predicts surrounding words given the current word.

https://arxiv.org/pdf/1301.3781.pdf

- Train latent-factors to solve one of these supervised learning tasks.

Word2Vec

- In both cases, each word i is represented by a vector z^i.
- We optimize likelihood of word vectors z^i under the model

$$p(x_i \mid x_{\text{nei}}) = \prod_{j \in \text{nei}} p(x_i \mid x_j), \quad p(x_i \mid x_j) \propto \frac{\exp(\langle z^i, z^j \rangle)}{\sum_{c=1}^{k} \exp(\langle z^c, z^j \rangle)}.$$

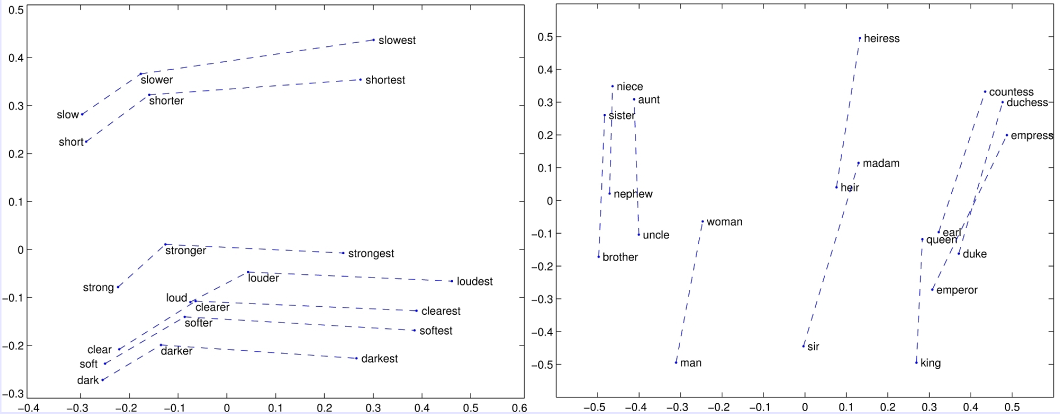
which is making a strong independence assumption.

- Apply gradient descent to NLL as usual:
  - Encourages $\langle z^i, z^j \rangle$ to be big for words in same context (making z^i close to z^j).
  - Encourages $\langle z^i, z^j \rangle$ to be small for words not appearing in same context.

- In CBOW, denominator sums over all words.
- In skip-grams, denominator sums over all possible surround words.
  - Common trick to speed things up:
    - Hierarchical softmax.
    - Negative sampling (sample terms in denominator).

Bonus Slide: Word2Vec

MDS visualization of a set of related words.



http://sebastianruder.com/secret-word2vec

Distances between vectors might represent semantic relationships.

Bonus Slide: Word2Vec

- Subtracting word vectors to find related words:

Table 8: *Examples of the word pair relationships, using the best word vectors from Table 4 (Skip-gram model trained on 783M words with 300 dimensionality).*

Relationship	Example 1	Example 2	Example 3
France - Paris	Italy: Rome	Japan: Tokyo	Florida: Tallahassee
big - bigger	small: larger	cold: colder	quick: quicker
Miami - Florida	Baltimore: Maryland	Dallas: Texas	Kona: Hawaii
Einstein - scientist	Messi: midfielder	Mozart: violinist	Picasso: painter
Sarkozy - France	Berlusconi: Italy	Merkel: Germany	Koizumi: Japan
copper - Cu	zinc: Zn	gold: Au	uranium: plutonium
Berlusconi - Silvio	Sarkozy: Nicolas	Putin: Medvedev	Obama: Barack
Microsoft - Windows	Google: Android	IBM: Linux	Apple: iPhone
Microsoft - Ballmer	Google: Yahoo	IBM: McNealy	Apple: Jobs
Japan - sushi	Germany: bratwurst	France: tapas	USA: pizza

Table 8 shows words that follow various relationships. We follow the approach described above: the relationship is defined by subtracting two word vectors, and the result is added to another word. Thus for example, *Paris* - *France* + *Italy* = *Rome*. As it can be seen, accuracy is quite good, although

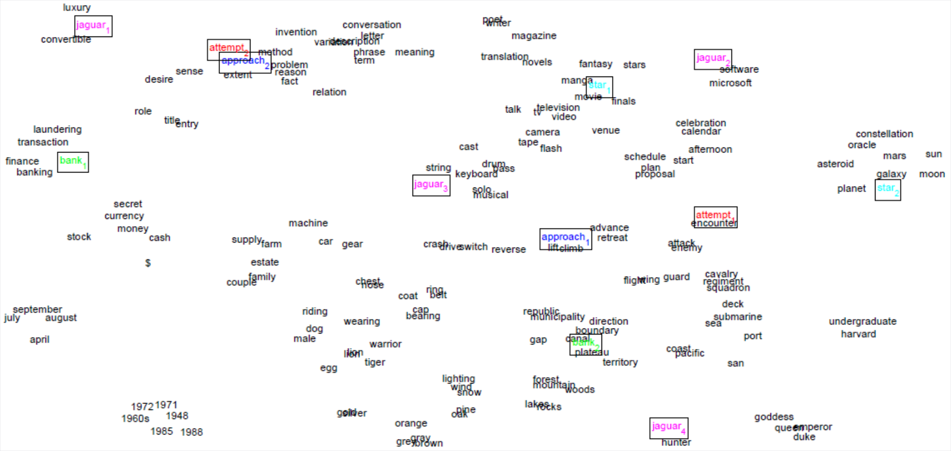
https://arxiv.org/pdf/1301.3781.pdf

- Word vectors for 157 languages:
  - https://fasttext.cc/docs/en/crawl-vectors.html

Multiple Word Prototypes

- What about homonyms and polysemy?
  - The word vectors would need to account for all meanings.
- More recent approaches:
  - Try to cluster the different context where words appear.
  - Use different vectors for different contexts.

Multiple Word Prototypes



http://www.socher.org/index.php/Main/ImprovingWordRepresentationsViaGlobalContextAndMultipleWordPrototypes