VARIATIONAL INFERENCE: FOUNDATIONS AND INNOVATIONS

David M. Blei
Departments of Computer Science and Statistics
Columbia University

The Buenos Aires Bleis

We have ***complicated data***; we want to ***make sense*** of it.

What is ***complicated data?***

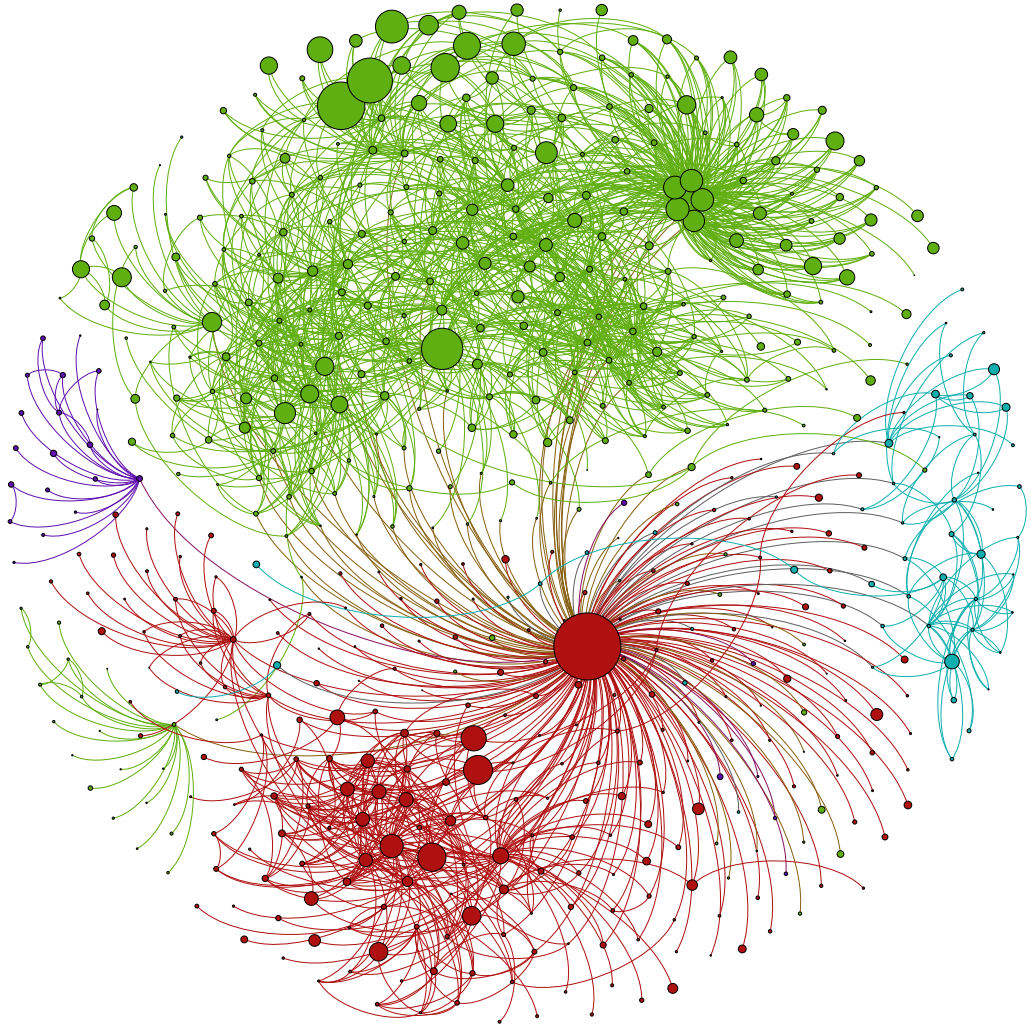
- many data points; many dimensions
- unstructured (e.g. text)
- multimodal and interconnected (e.g., images, links, text, clicks)

What is ***making sense of data***?

- make predictions about the future
- identify interpretable patterns
- do science: confirm, elaborate, form causal theories

PROBABILISTIC MACHINE LEARNING

- ML methods that *connect domain knowledge to data*.
- Provides a computational methodology for scalable modeling
- Goal: A methodology that is *expressive, scalable, easy to develop*

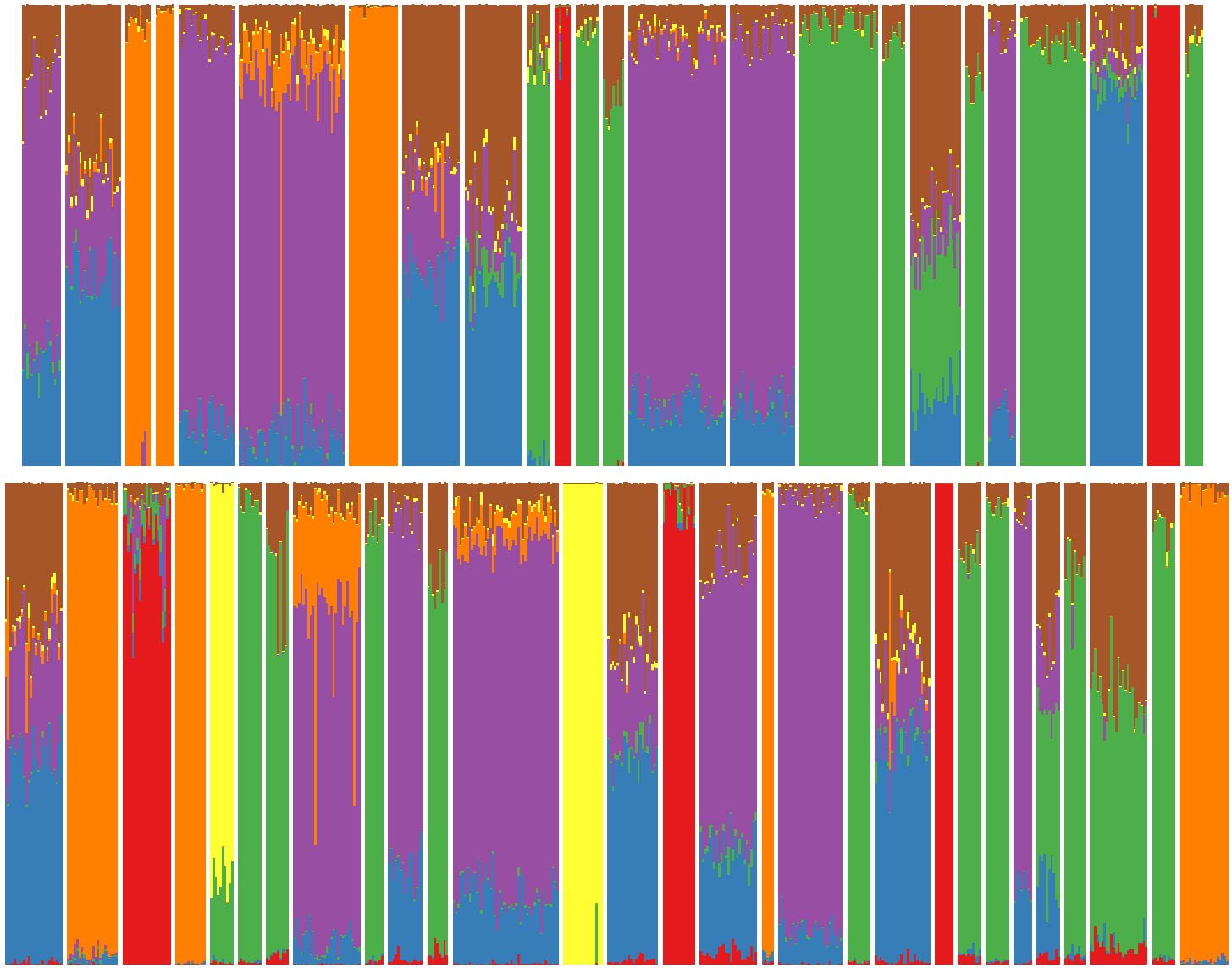


Communities discovered in a 3.7M node network of U.S. Patents

[Gopalan and Blei PNAS 2013]

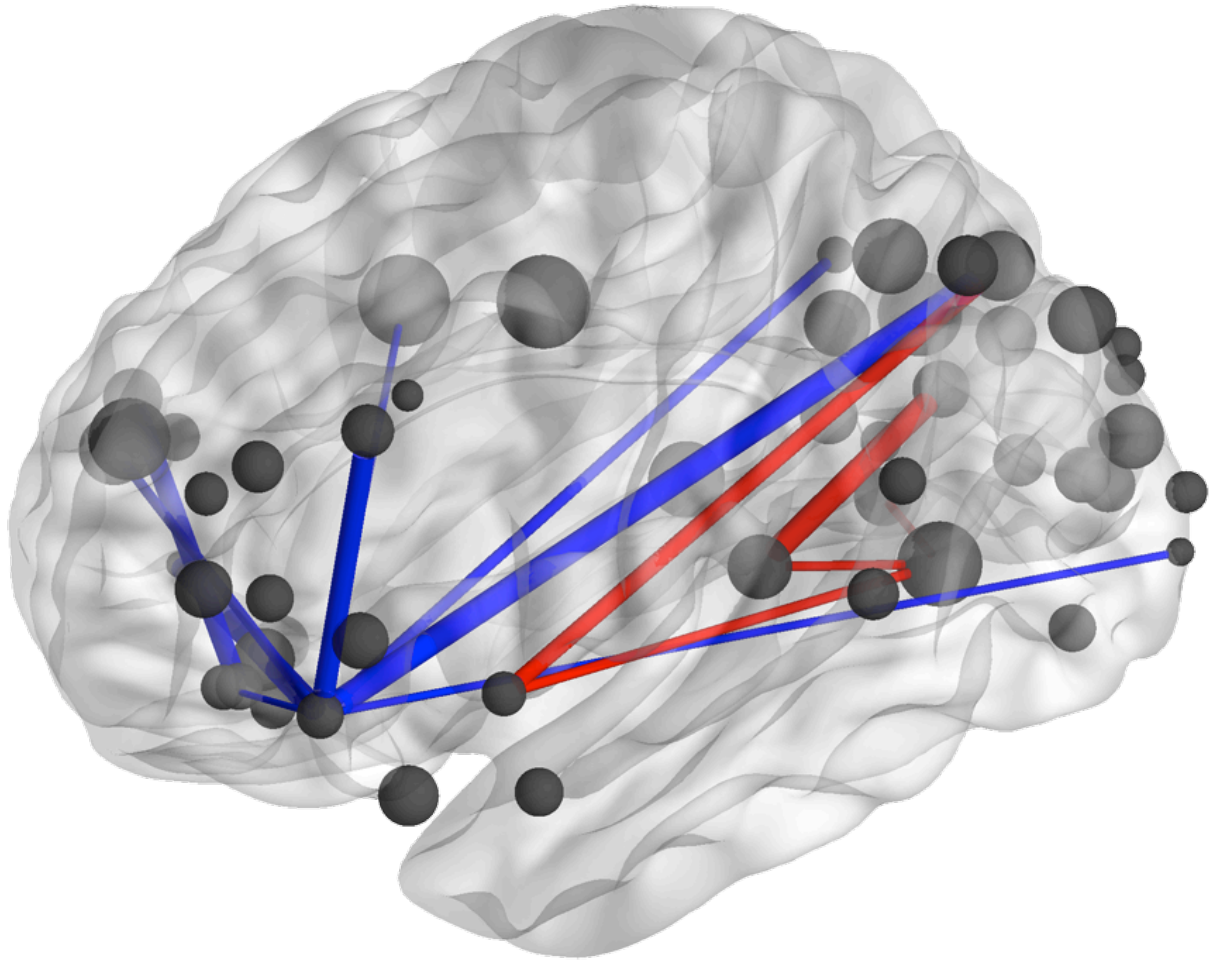
Topics found in 1.8M articles from the New York Times

[Hoffman+ JMLR 2013]



Population analysis of 2 billion genetic measurements

[Gopalan+ Nature Genetics 2016]

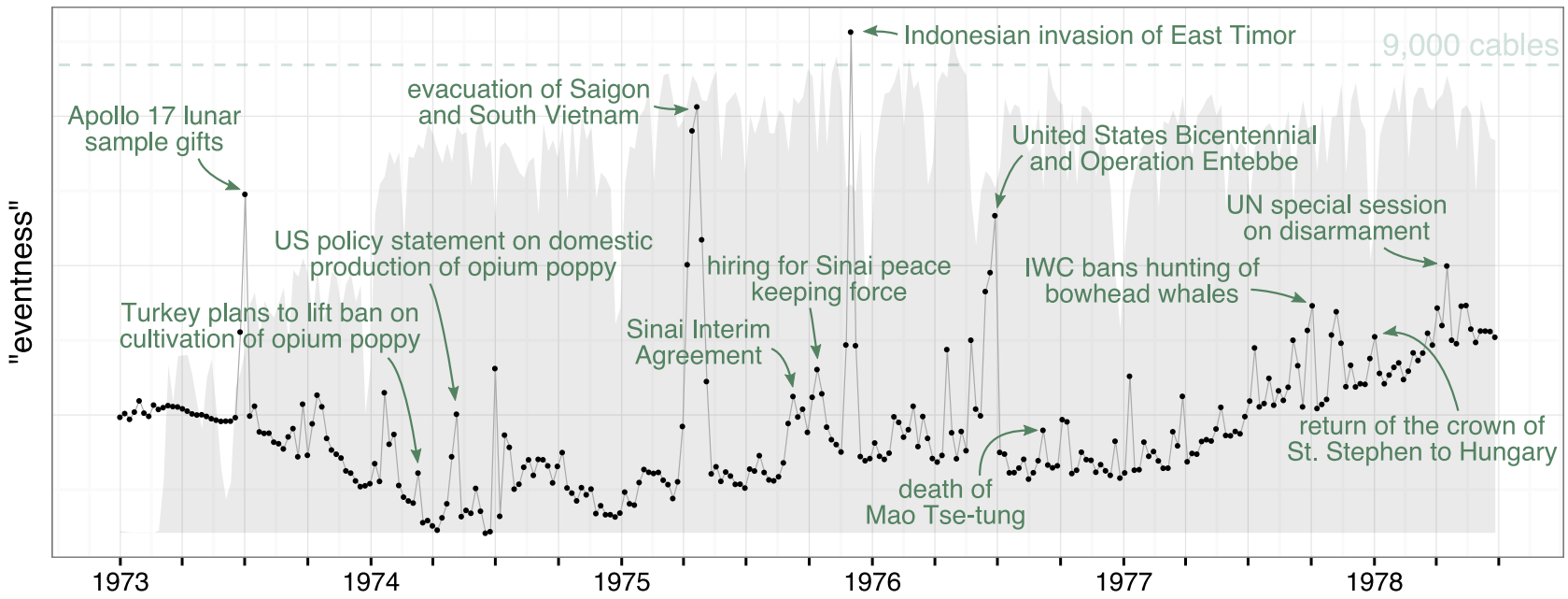


Neuroscience analysis of 220 million fMRI measurements

[Manning+ PLOS ONE 2014]

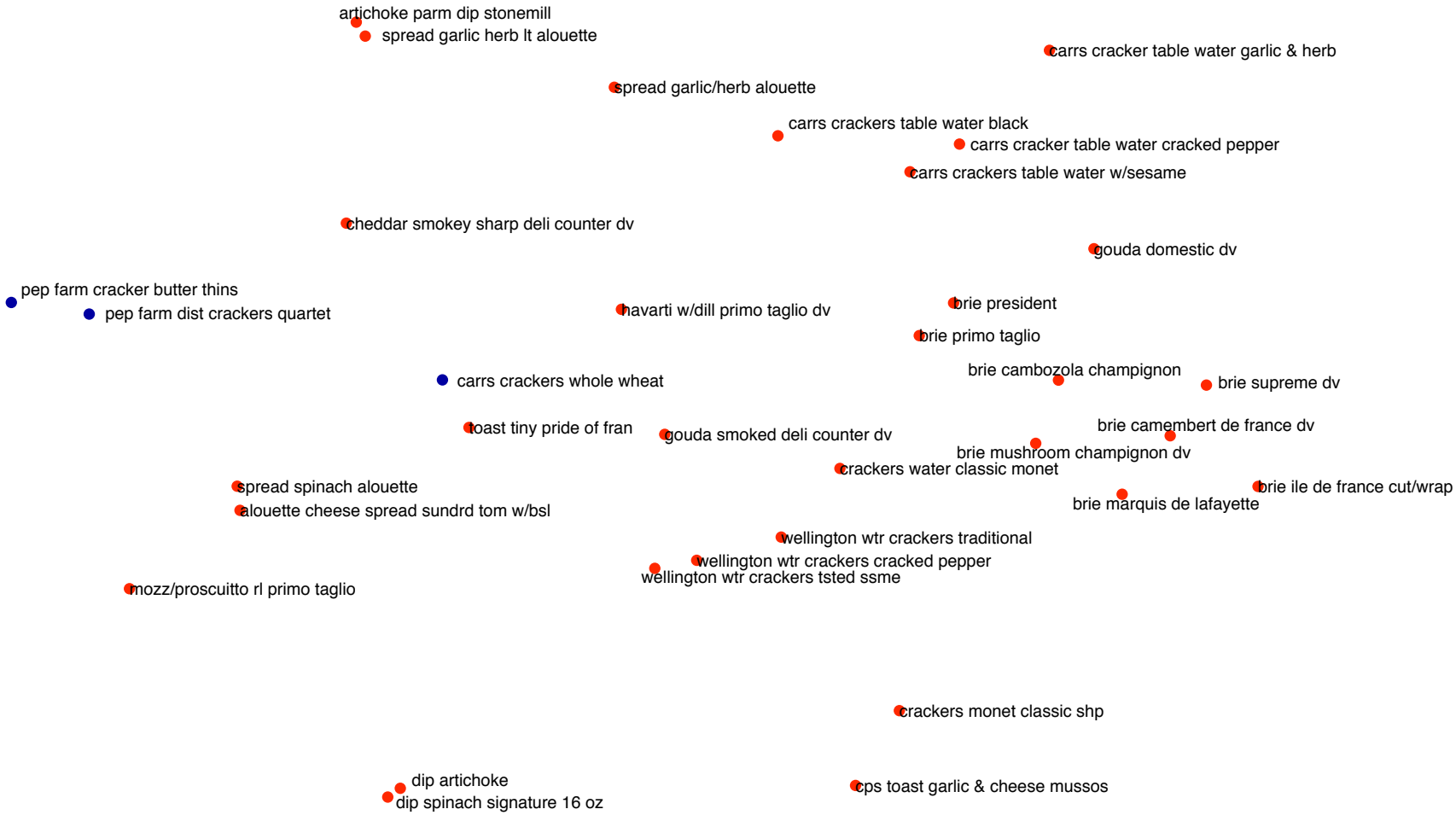
Analysis of 1.7M taxi trajectories, in Stan

[Kucukelbir+ JMLR 2016]



Analysis of 2M declassified cables from the State Dept

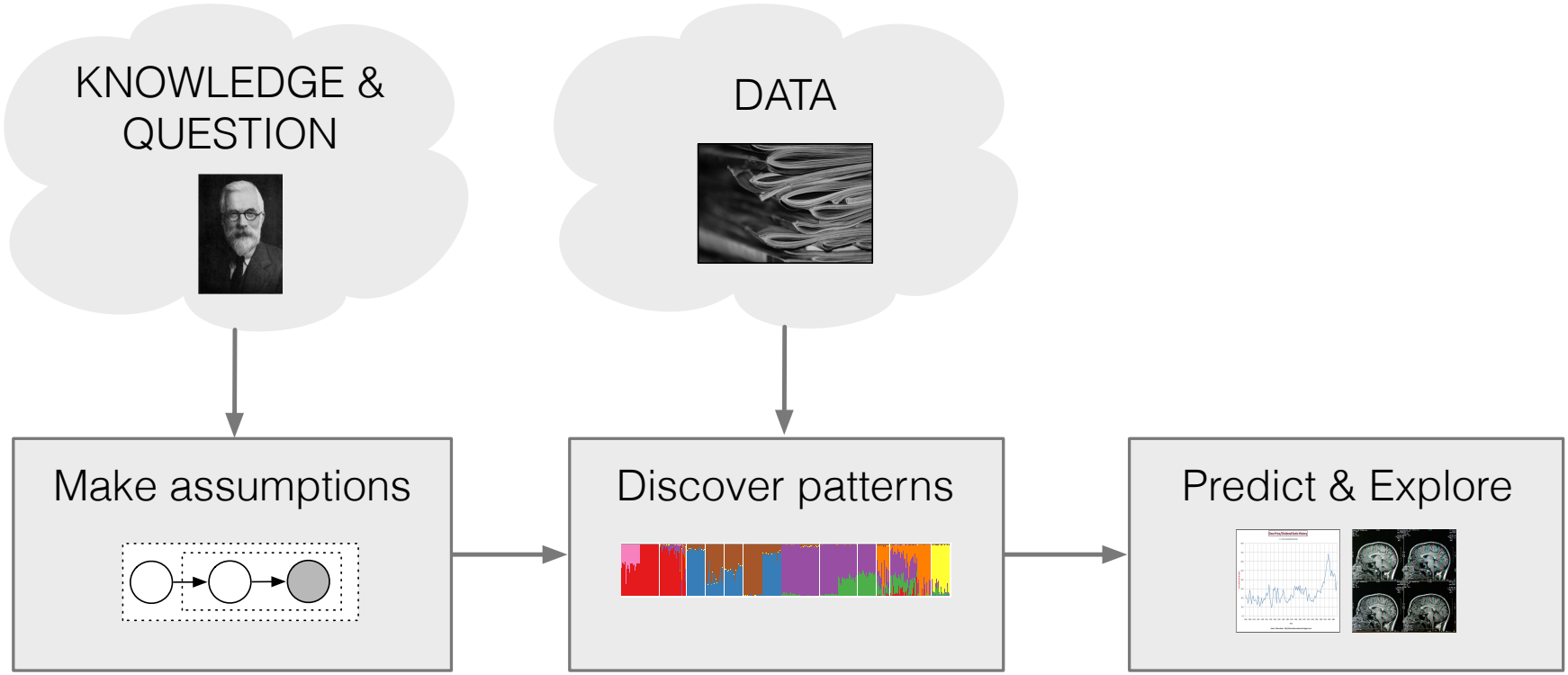
[Chaney+ EMNLP 2016]



(Fancy) discrete choice analysis of 5.7M purchases

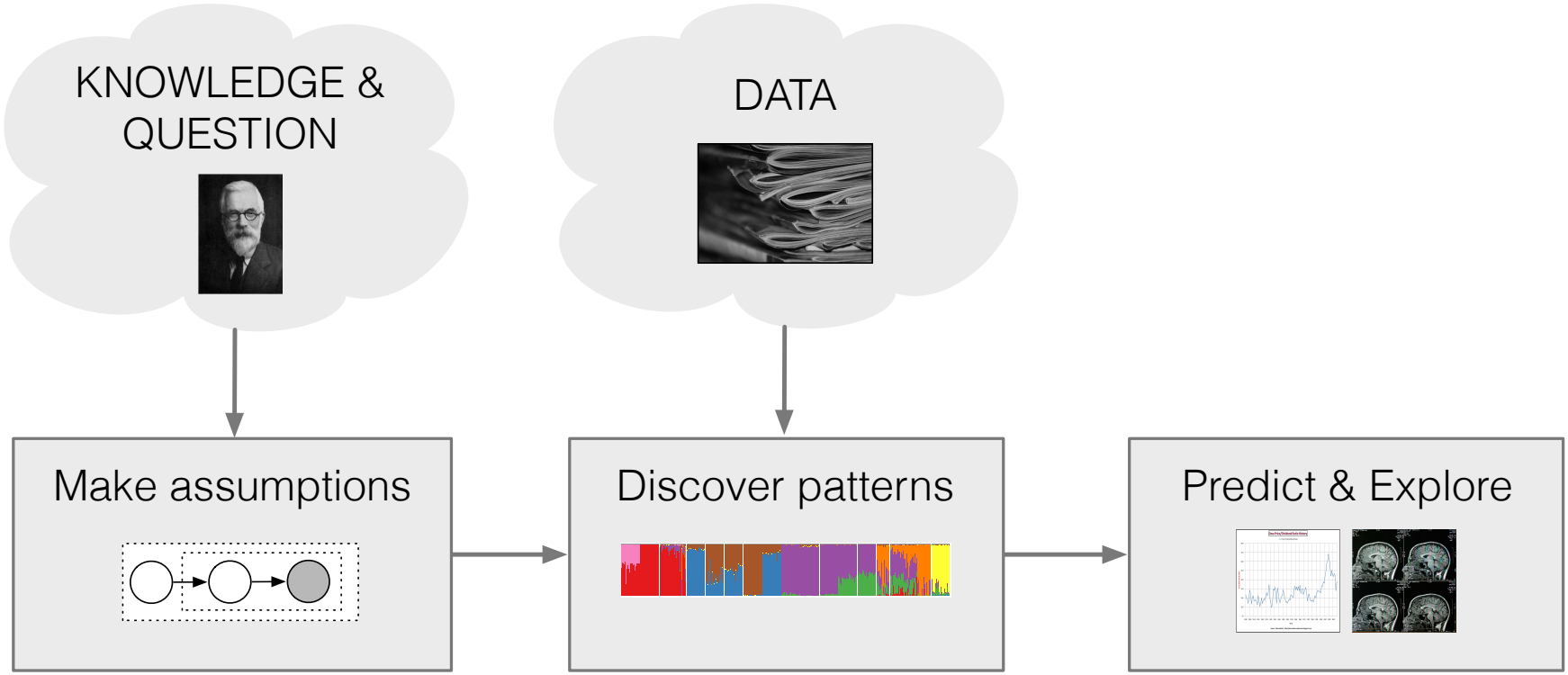
[Ruiz+ 2017]

The probabilistic pipeline

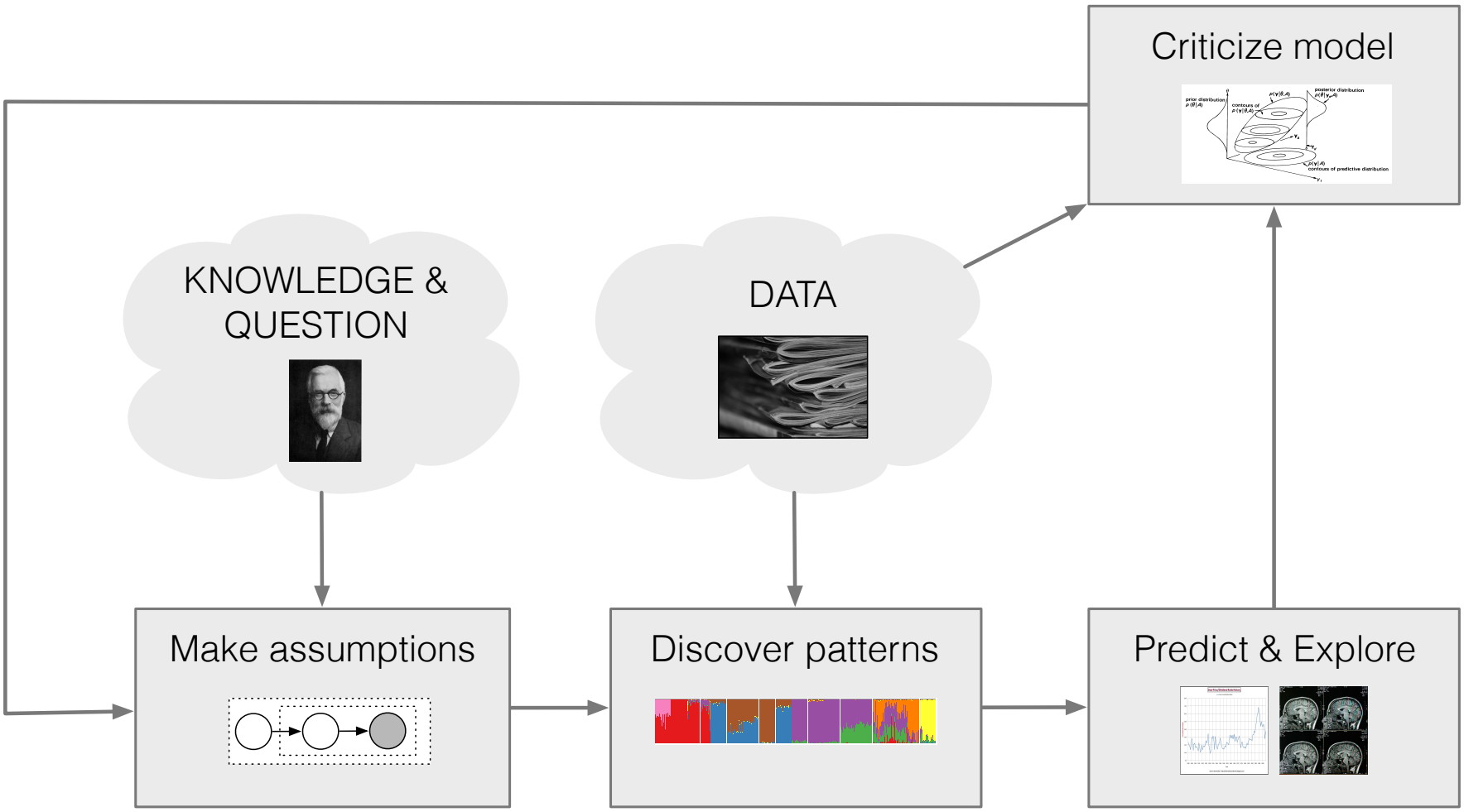


- Customized data analysis is important to many fields.
- Pipeline separates **assumptions**, **computation**, **application**
- Eases collaborative solutions to statistics problems

The probabilistic pipeline



- **Posterior inference** is the key algorithmic problem.
- Answers the question: What does this model say about this data?
- Goal: **General** and **scalable** approaches to posterior inference



[Box, 1980; Rubin, 1984; Gelman+ 1996; Blei, 2014]

Introduction

Probabilistic machine learning

- A probabilistic model is a joint distribution of hidden variables $\mathbf{z}$ and observed variables $\mathbf{x}$,

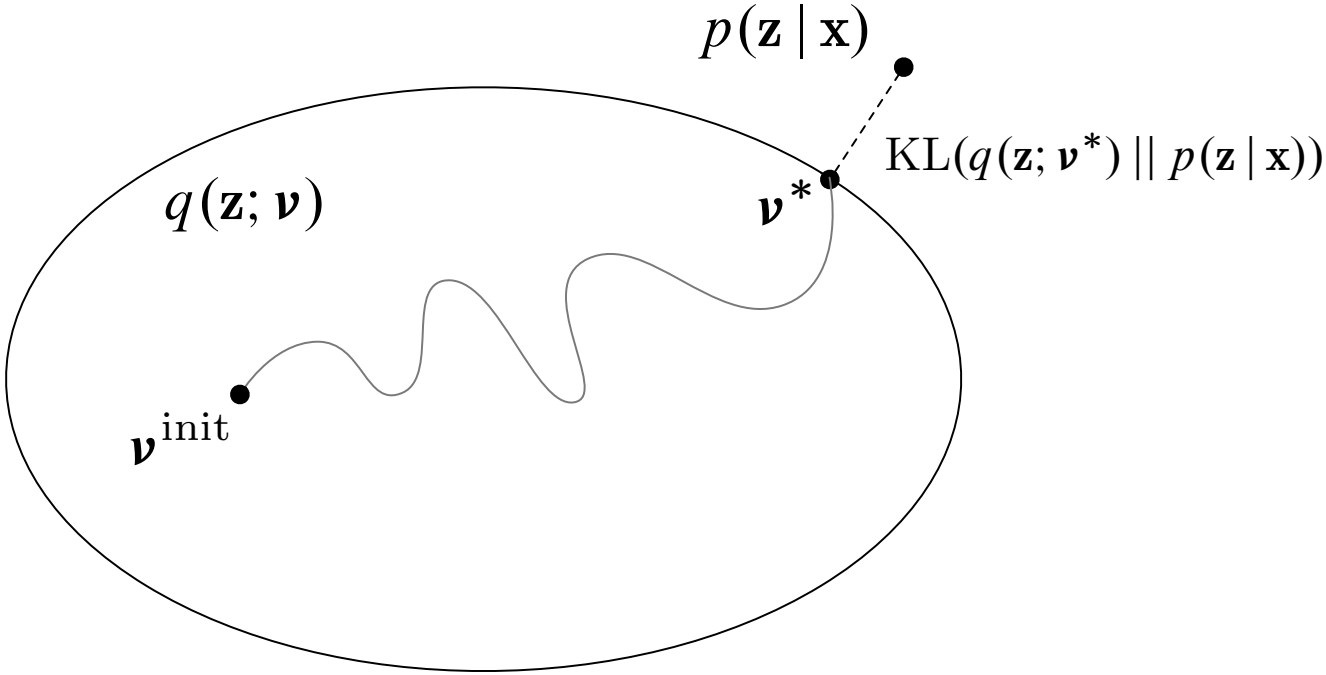
$$p(\mathbf{z}, \mathbf{x}).$$

- Inference about the unknowns is through the **posterior**, the conditional distribution of the hidden variables given the observations

$$p(\mathbf{z} \mid \mathbf{x}) = \frac{p(\mathbf{z}, \mathbf{x})}{p(\mathbf{x})}.$$

- For most interesting models, the denominator is not tractable.
  We appeal to **approximate posterior inference**.

Variational inference

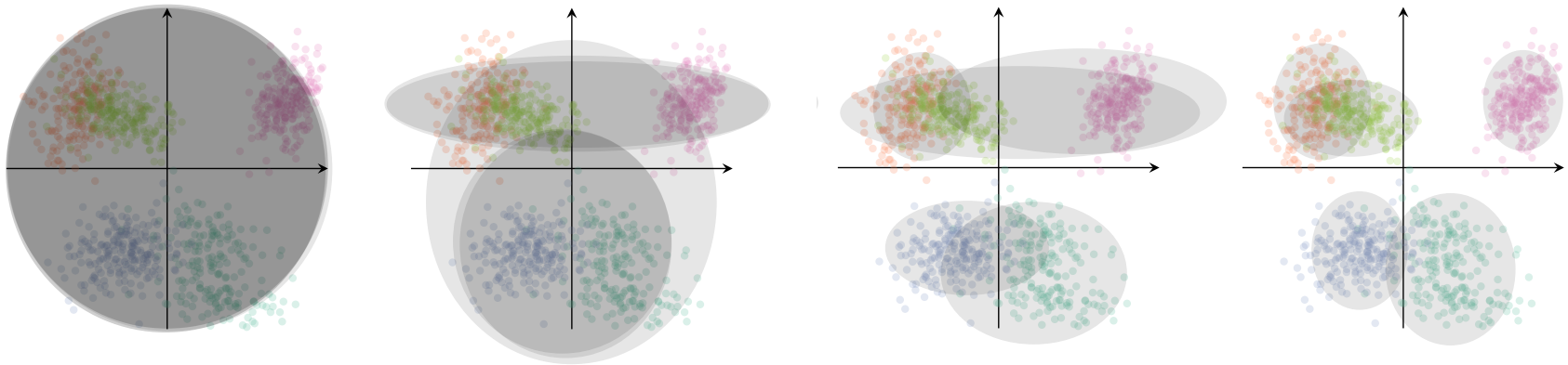


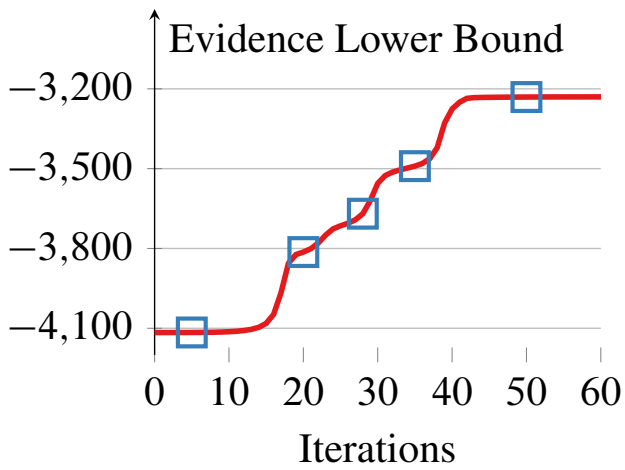
- VI solves **inference** with **optimization**.
  (Contrast this with MCMC.)
- Posit a **variational family** of distributions over the latent variables,

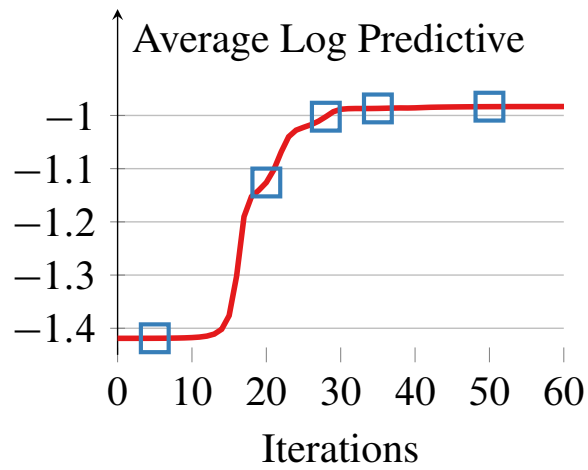
$$q(\mathbf{z}; \boldsymbol{\nu})$$

- Fit the **variational parameters** $\boldsymbol{\nu}$ to be close (in KL) to the exact posterior.
  (There are alternative divergences, which connect to algorithms like EP, BP, and others.)

Example: Mixture of Gaussians

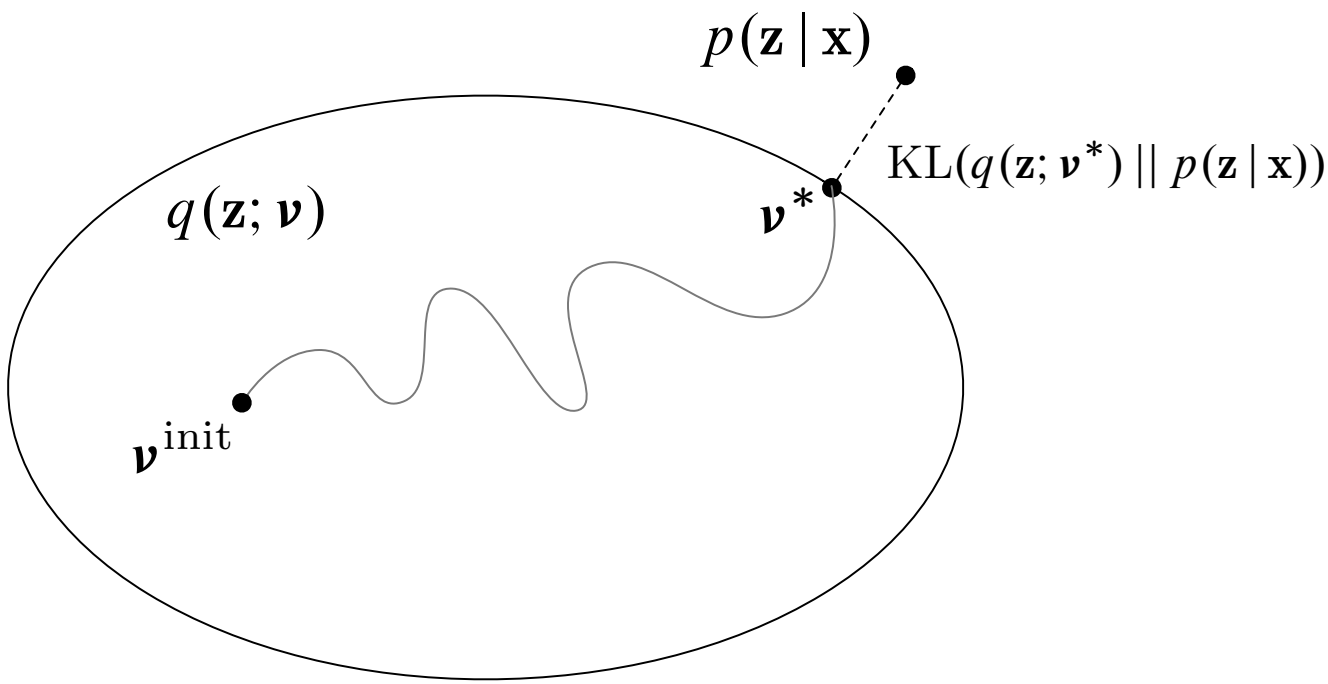






[images by Alp Kucukelbir; Blei+ 2016]

Variational inference



VI solves **inference** with **optimization**.

In this tutorial:

- the **basics** of VI
- VI for **massive data**
- VI for a wide class of **difficult models**

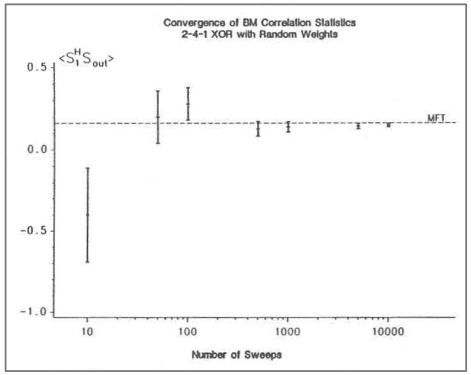
“Prerequisites”

- A little probability
  - joint distribution, conditional distribution
  - expectation, conditional expectation
- A little optimization
  - the main idea
  - gradient-based optimization
  - coordinate-ascent optimization
- A little Bayesian statistics (but you don’t have to be a Bayesian!)

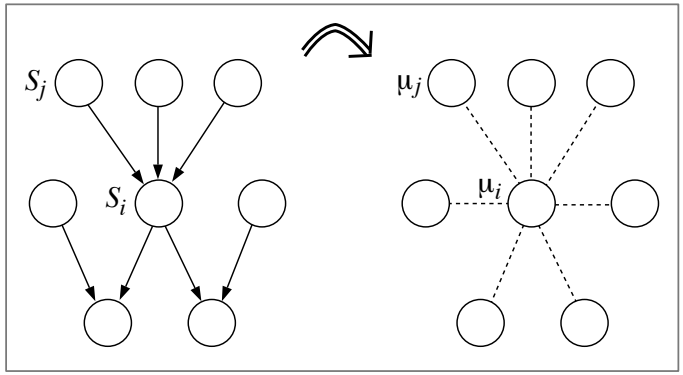
What you will learn about

- The basics of variational inference (VI)
  - Mean-field variational inference
  - Coordinate ascent optimization for VI
- Stochastic variational inference for massive data
- Black box variational inference
  - Score gradients
  - Reparameterization gradients
  - Amortized variational families, the variational autoencoder
  - Probabilistic programming
- Models, along the way
  - Latent Dirichlet allocation and topic models
  - Deep exponential families
  - Embedding models of consumer behavior
  - Deep generative models

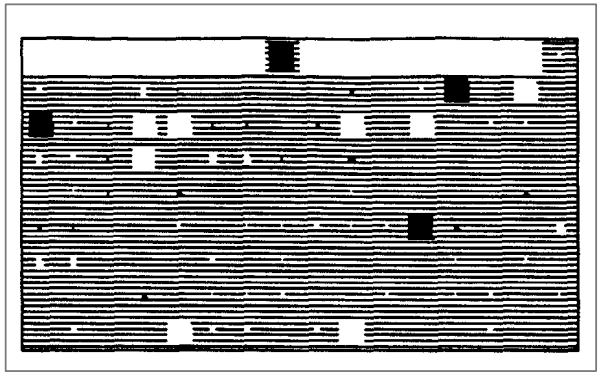
History



[Peterson and Anderson 1987]



[Jordan et al. 1999]

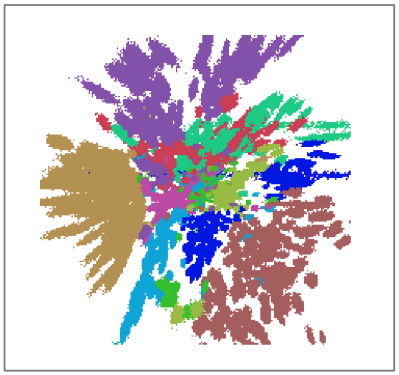


[Hinton and van Camp 1993]

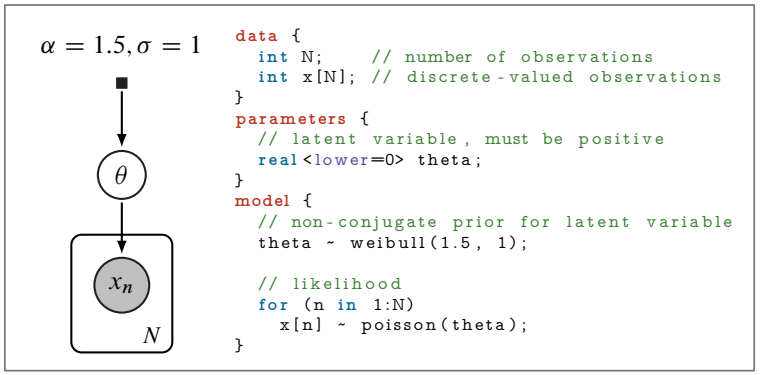
- Variational inference (VI) adapts **ideas from statistical physics** to probabilistic inference. Arguably, it began in the late eighties with Peterson and Anderson (1987), who fit a neural network with mean-field methods.
- This idea was picked up by Jordan's lab in the early 1990s—Tommi Jaakkola, Lawrence Saul, Zoubin Ghahramani—who **generalized it to many probabilistic models**. (A review paper is Jordan+ 1999.)
- Hinton and Van Camp (1993) also developed **mean-field methods for neural networks**. Neal and Hinton (1993) connected VI to EM, which lead to VI for mixtures of experts (Waterhouse+ 1996), HMMs (MacKay, 1997), and more neural networks (Barber and Bishop, 1998).

Today

[Kingma and Welling 2013]



[Rezende et al. 2014]

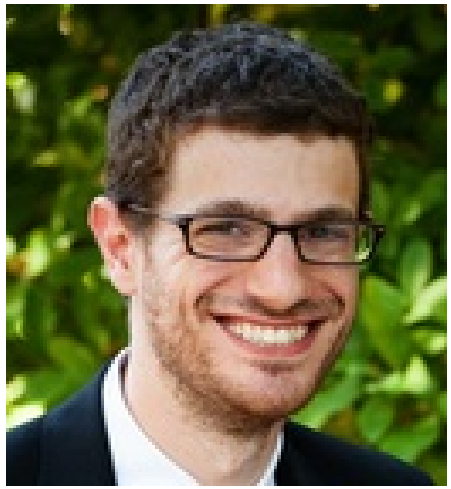


[Kucukelbir et al. 2015]

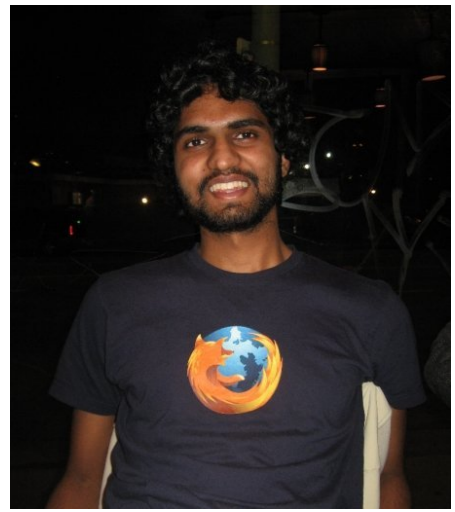
- There is now a flurry of new work on variational inference, making it *scalable*, *easier to derive*, *faster*, and *more accurate*.

- VI touches many areas: probabilistic programming, reinforcement learning, neural networks, convex optimization, and Bayesian statistics.

Collaborators



Matt Hoffman
(Google)

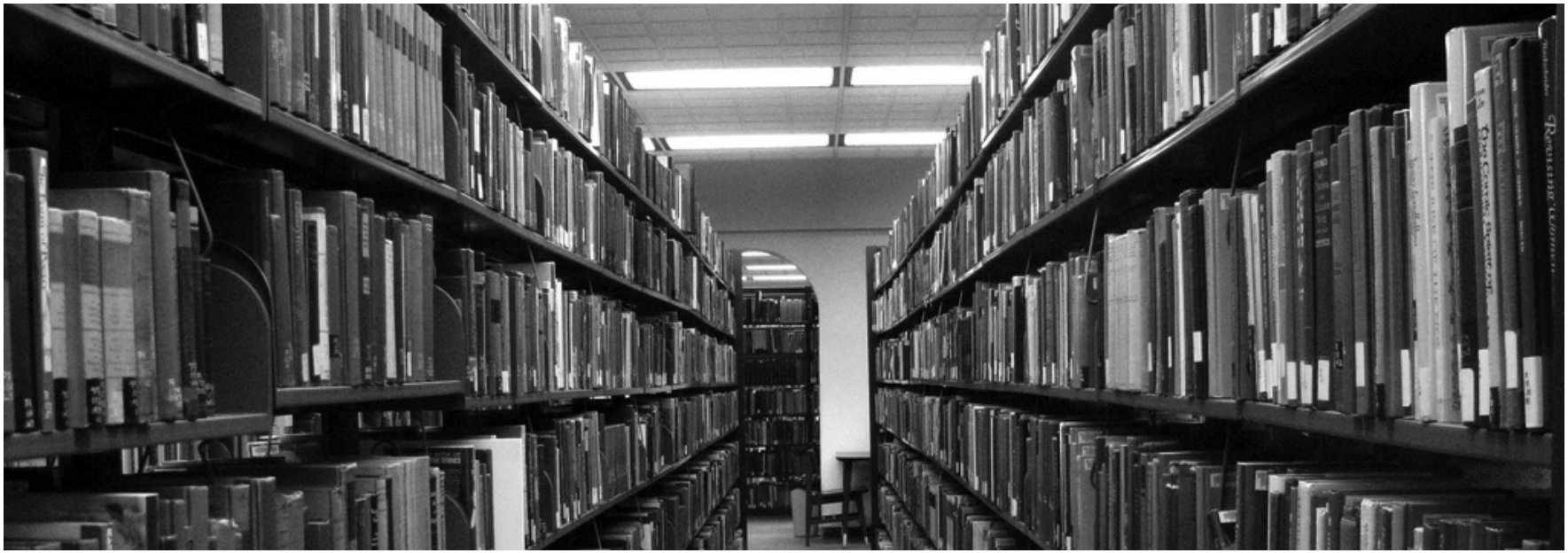


Rajesh Ranganath
(NYU)

Alp Kucukelbir
(Fero Labs)

Variational Inference
& Stochastic Variational Inference

Motivation: Topic Modeling



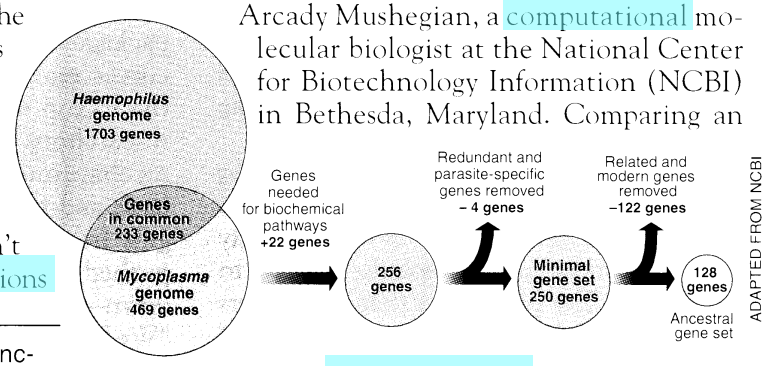
Topic models use posterior inference to discover the hidden thematic structure in a large collection of documents.

Example: Latent Dirichlet Allocation (LDA)

Seeking Life's Bare (Genetic) Necessities

COLD SPRING HARBOR, NEW YORK—How many genes does an organism need to survive? Last week at the genome meeting here,* two genome researchers with radically different approaches presented complementary views of the basic genes needed for life. One research team, using computer analyses to compare known genomes, concluded that today's organisms can be sustained with just 250 genes, and that the earliest life forms required a mere 128 genes. The other researcher mapped genes in a simple parasite and estimated that for this organism, 800 genes are plenty to do the job—but that anything short of 100 wouldn't be enough.

Although the numbers don't match precisely, those predictions "are not all that far apart," especially in comparison to the 75,000 genes in the human genome, notes Siv Andersson of Uppsala University in Sweden, who arrived at the 800 number. But coming up with a consensus answer may be more than just a genetic numbers game, particularly as more and more genomes are completely mapped and sequenced. "It may be a way of organizing any newly sequenced genome," explains Arcady Mushegian, a computational molecular biologist at the National Center for Biotechnology Information (NCBI) in Bethesda, Maryland. Comparing an



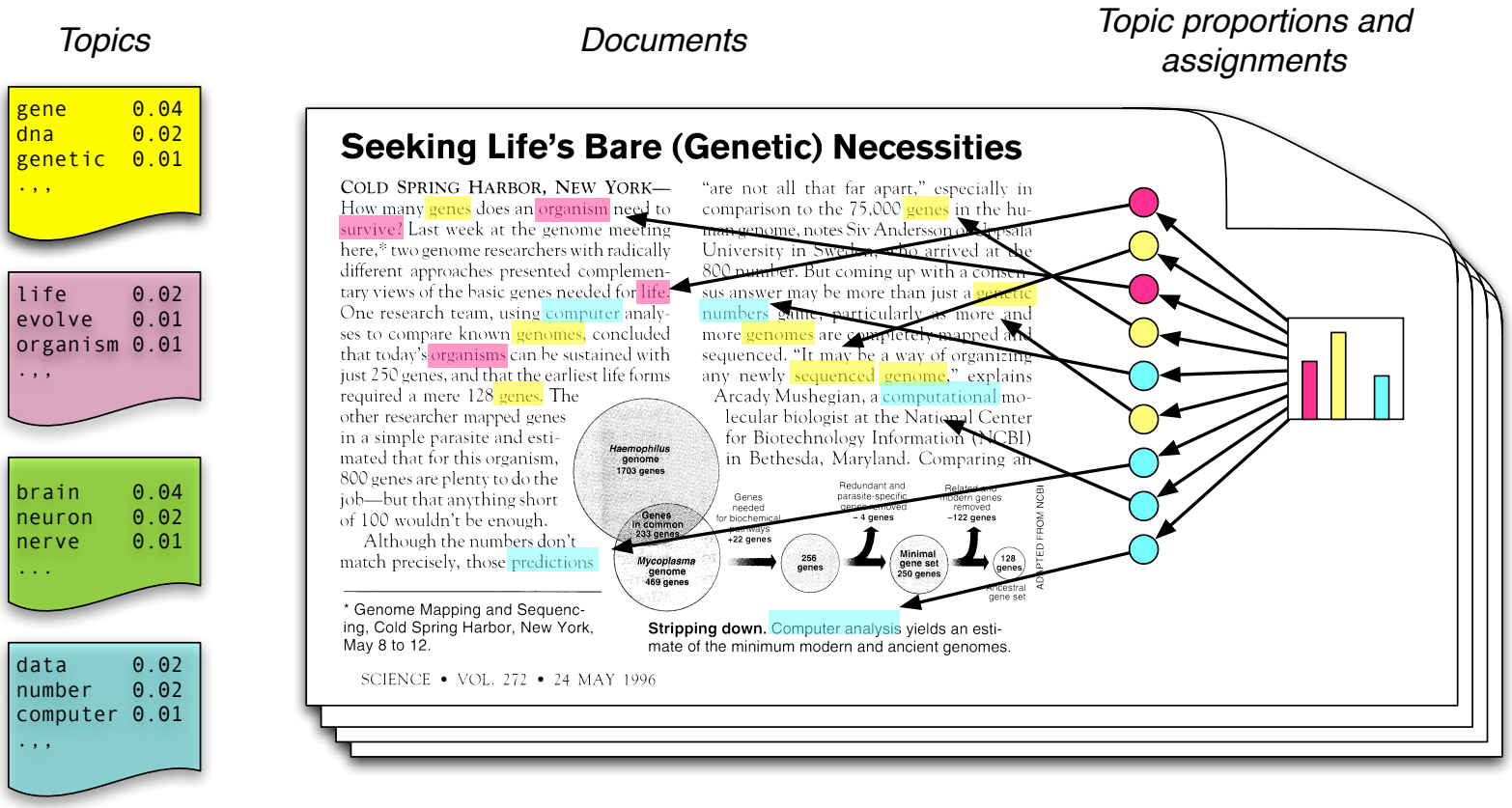
Stripping down. Computer analysis yields an estimate of the minimum modern and ancient genomes.

* Genome Mapping and Sequencing, Cold Spring Harbor, New York, May 8 to 12.

SCIENCE • VOL. 272 • 24 MAY 1996

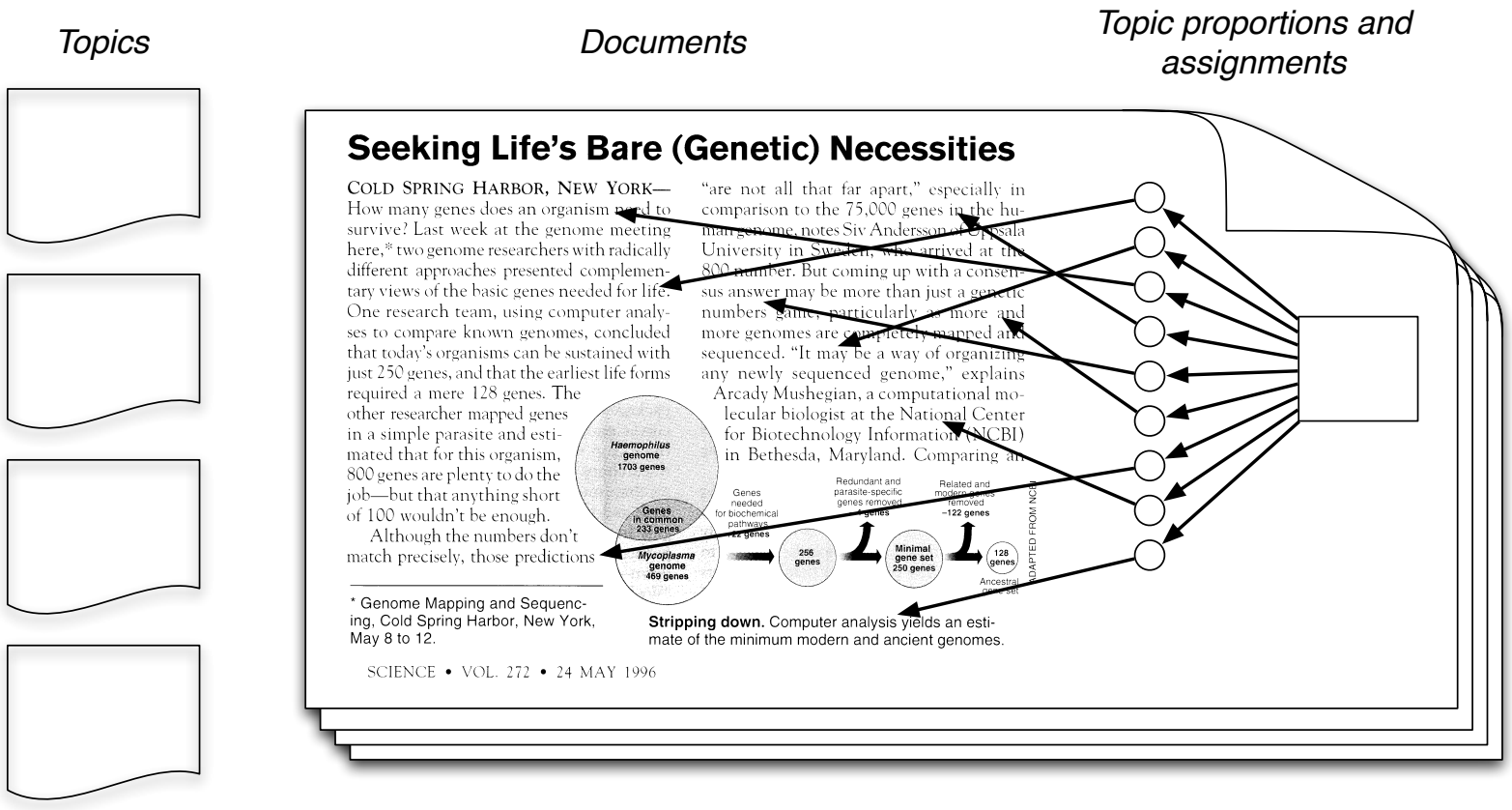
Documents exhibit multiple topics.

Example: Latent Dirichlet Allocation (LDA)



- Each **topic** is a distribution over words
- Each **document** is a mixture of corpus-wide topics
- Each **word** is drawn from one of those topics

Example: Latent Dirichlet Allocation (LDA)

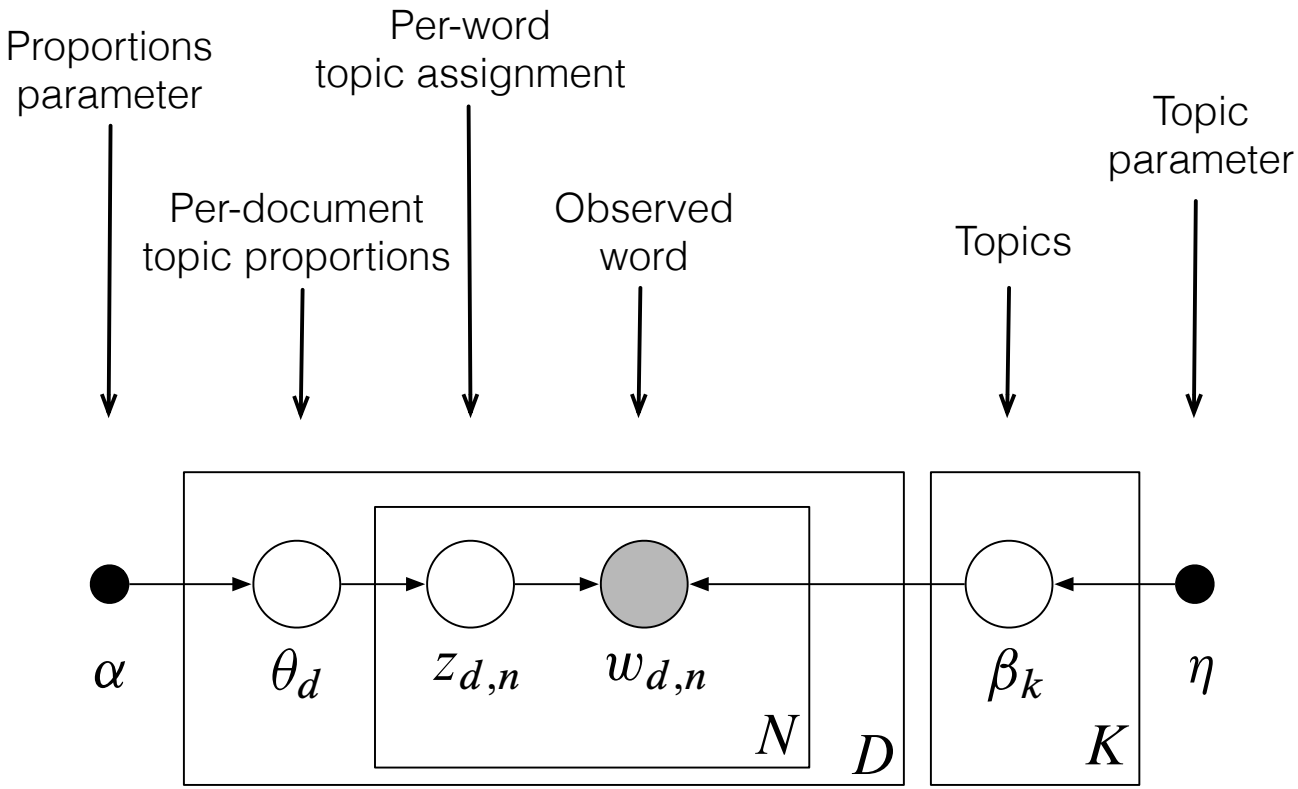


- But we only observe the documents; everything else is hidden.
- So we want to calculate the posterior

$$p(\text{topics, proportions, assignments} \mid \text{documents})$$

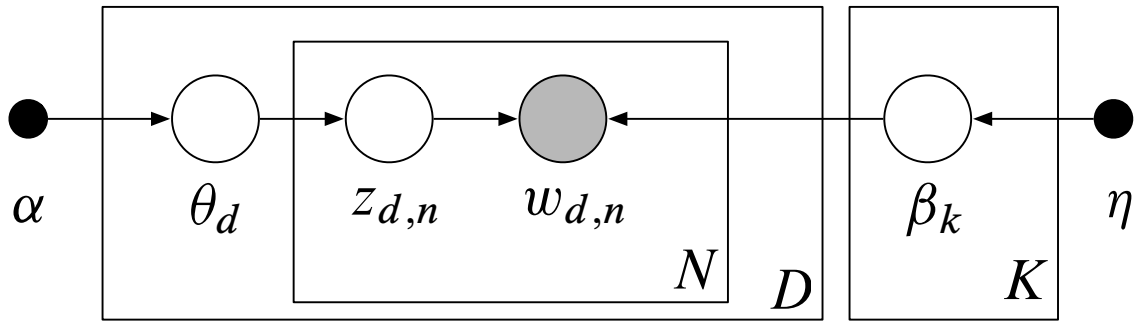
(Note: millions of documents; billions of latent variables)

LDA as a Graphical Model



- Encodes **assumptions** about data with a factorization of the joint
- Connects assumptions to **algorithms** for computing with data
- Defines the **posterior** (through the joint)

Posterior Inference



- The posterior of the latent variables given the documents is

$$p(\beta, \boldsymbol{\theta}, \mathbf{z} \mid \mathbf{w}) = \frac{p(\beta, \boldsymbol{\theta}, \mathbf{z}, \mathbf{w})}{\int_\beta \int_{\boldsymbol{\theta}} \sum_{\mathbf{z}} p(\beta, \boldsymbol{\theta}, \mathbf{z}, \mathbf{w})}.$$

- We can't compute the denominator, the marginal $p(\mathbf{w})$.
- We use approximate inference.

Mean-field variational inference for LDA

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COLD SPRING HARBOR, NEW YORK—How many genes does an organism need to survive? Last week at the genome meeting here,* two genome researchers with radically different approaches presented complementary views of the basic genes needed for life. One research team, using computer analyses to compare known genomes, concluded that today's organisms can be sustained with just 250 genes, and that the earliest life forms required a mere 128 genes. The other researcher mapped genes in a simple parasite and estimated that for this organism, 800 genes are plenty to do the job—but that anything short of 100 wouldn't be enough.

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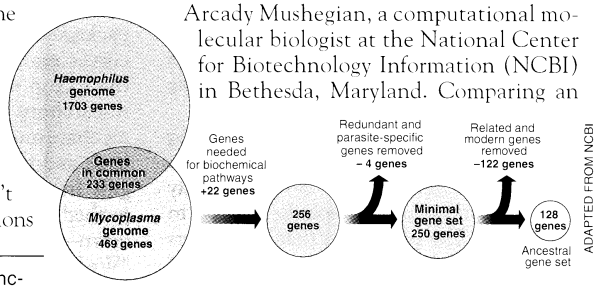

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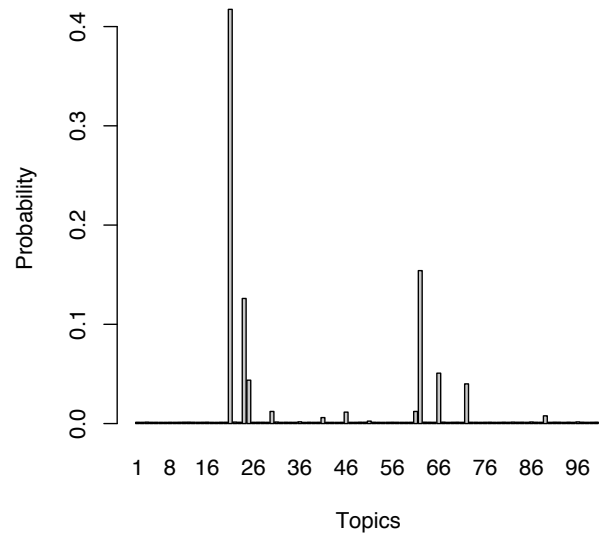
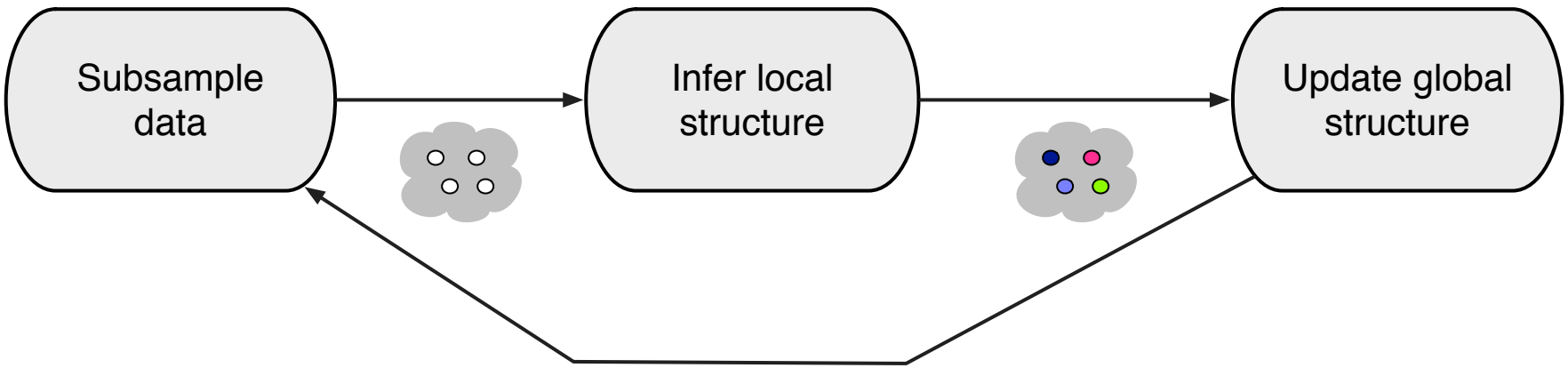


Mean-field variational inference for LDA

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

Topics found in 1.8M articles from the New York Times

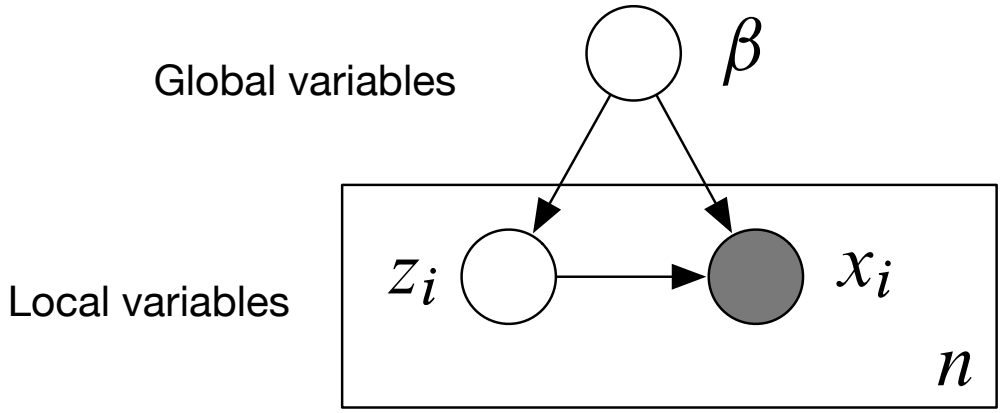
Mean-field VI and Stochastic VI



Road map:

- Define the generic class of conditionally conjugate models
- Derive classical mean-field VI
- Derive stochastic VI, which scales to massive data

Conditionally conjugate models

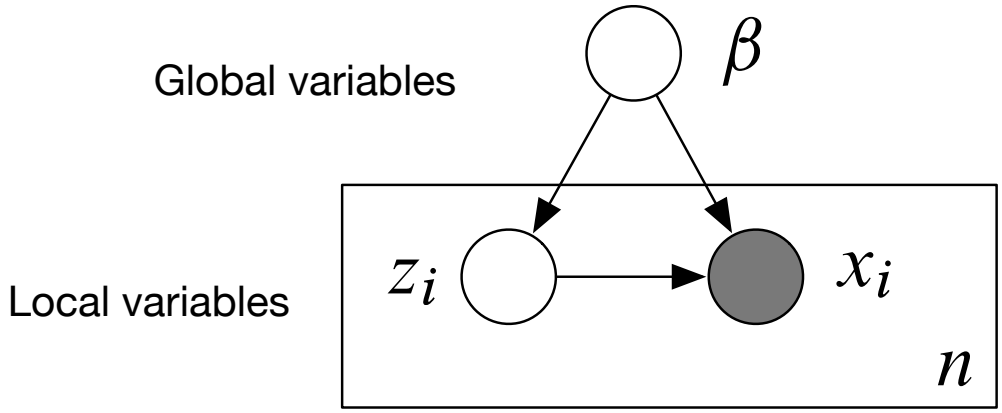


$$p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^{n} p(z_i, x_i \mid \beta)$$

- The observations are $\mathbf{x} = x_{1:n}$.
- The **local** variables are $\mathbf{z} = z_{1:n}$.
- The **global** variables are β.
- The ith data point x_i only depends on z_i and β.

Compute $p(\beta, \mathbf{z} \mid \mathbf{x})$.

Conditionally conjugate models



$$p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^{n} p(z_i, x_i \mid \beta)$$

- A **complete conditional** is the conditional of a latent variable given the observations and other latent variables.
- Assume each complete conditional is in the exponential family,

$$p(z_i \mid \beta, x_i) = h(z_i) \exp\{\eta_\ell(\beta, x_i)^\top z_i - a(\eta_\ell(\beta, x_i))\}$$
$$p(\beta \mid \mathbf{z}, \mathbf{x}) = h(\beta) \exp\{\eta_g(\mathbf{z}, \mathbf{x})^\top \beta - a(\eta_g(\mathbf{z}, \mathbf{x}))\}.$$

(The exponential family include most distributions that we use.)

Aside: The exponential family

$$p(x) = h(x) \exp\{\eta^\top t(x) - a(\eta)\}$$

Terminology:

η	the natural parameter
$t(x)$	the sufficient statistics
$a(\eta)$	the log normalizer
$h(x)$	the underlying measure (not important)

Aside: The exponential family

$$p(x) = h(x) \exp\{\eta^\top t(x) - a(\eta)\}$$

- The log normalizer is

$$a(\eta) = \log \int \exp\{\eta^\top t(x)\} dx$$

- It ensures the density integrates to one.
- Its gradient calculates the expected sufficient statistics

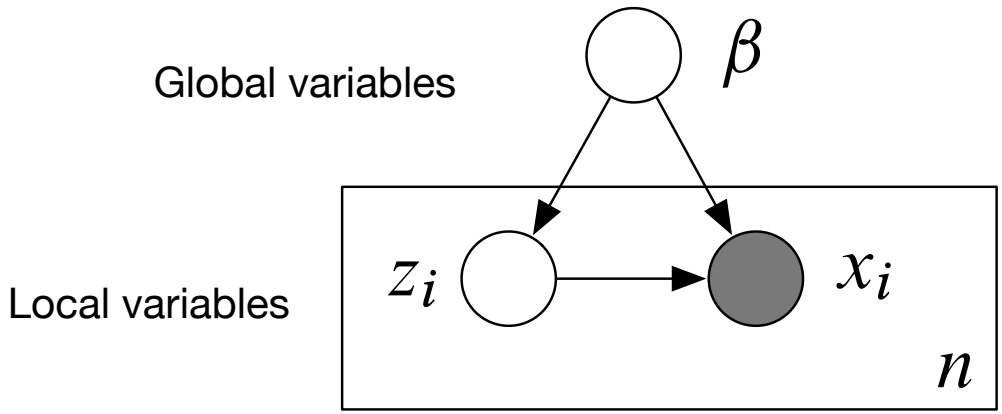
$$\mathbb{E}[X] = \nabla_\eta a(\eta).$$

Aside: The exponential family

$$p(x) = h(x) \exp\{\eta^\top t(x) - a(\eta)\}$$

- Many common distributions are in the exponential family—
  Bernoulli, categorical, Gaussian, Poisson, Beta, Dirichlet, Gamma, etc.
- Outlines the theory around conjugate priors and corresponding posteriors
- Connects closely to variational inference [Wainwright and Jordan, 2008]

Conditionally conjugate models



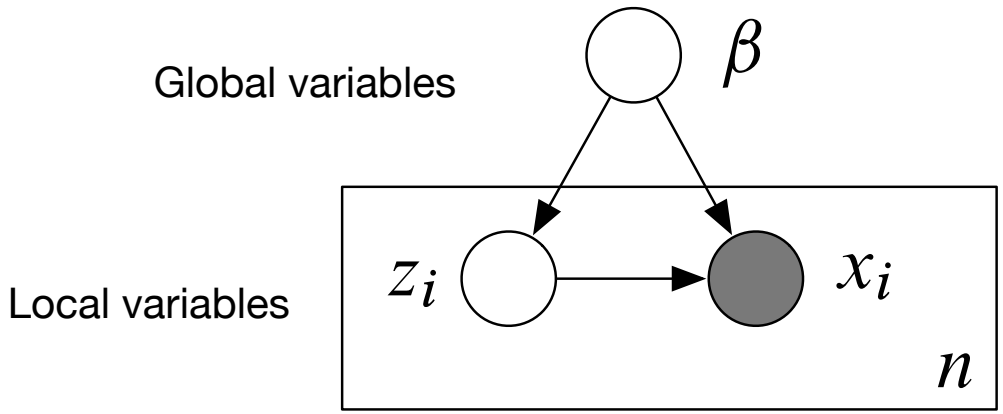
$$p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^{n} p(z_i, x_i \mid \beta)$$

- A **complete conditional** is the conditional of a latent variable given the observations and other latent variable.
- The global parameter comes from conjugacy [Bernardo and Smith, 1994]

$$\eta_g(\mathbf{z}, \mathbf{x}) = \alpha + \sum_{i=1}^{n} t(z_i, x_i),$$

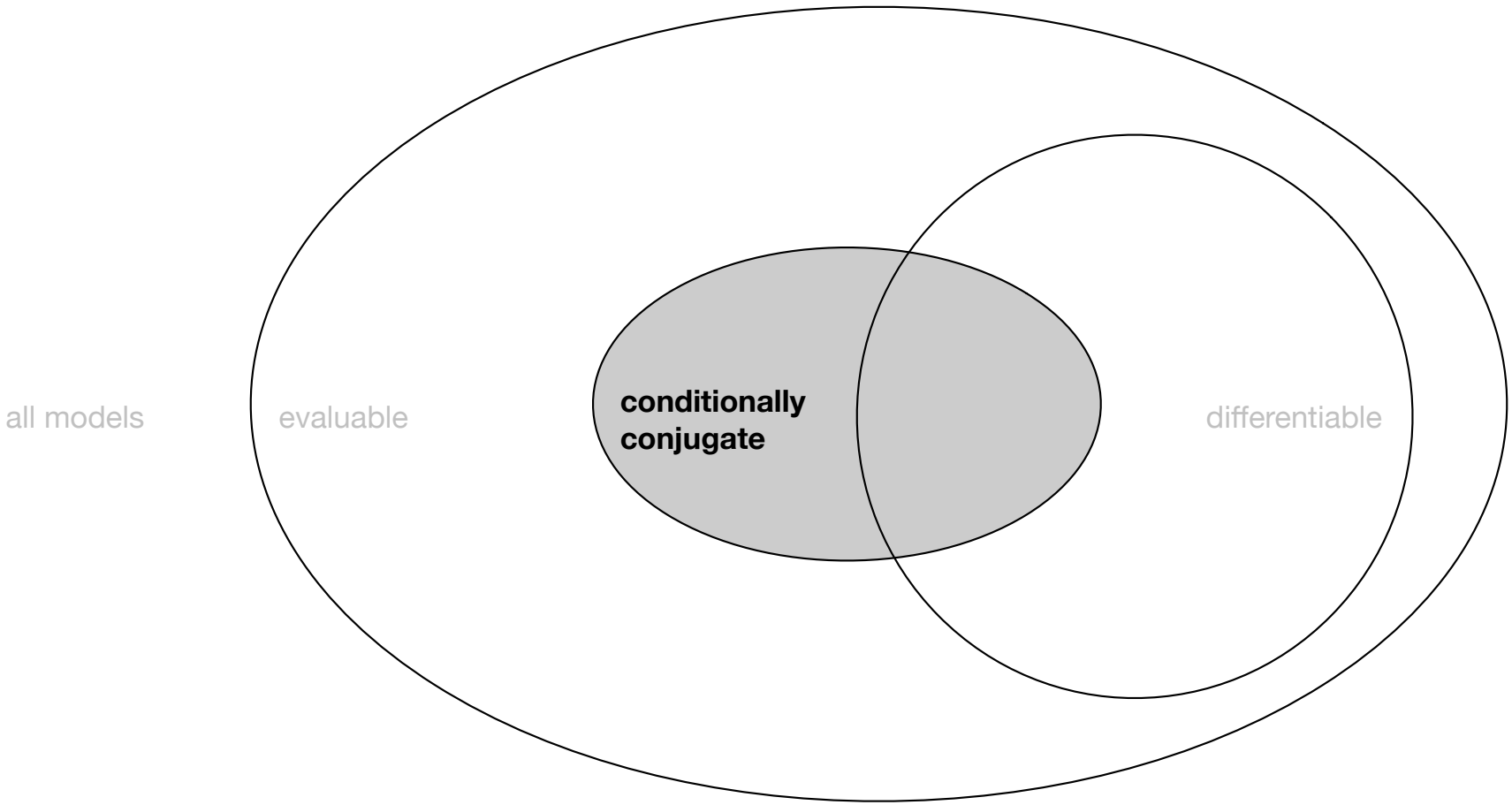
where α is a hyperparameter and $t(\cdot)$ are sufficient statistics for $[z_i, x_i]$.

Conditionally conjugate models

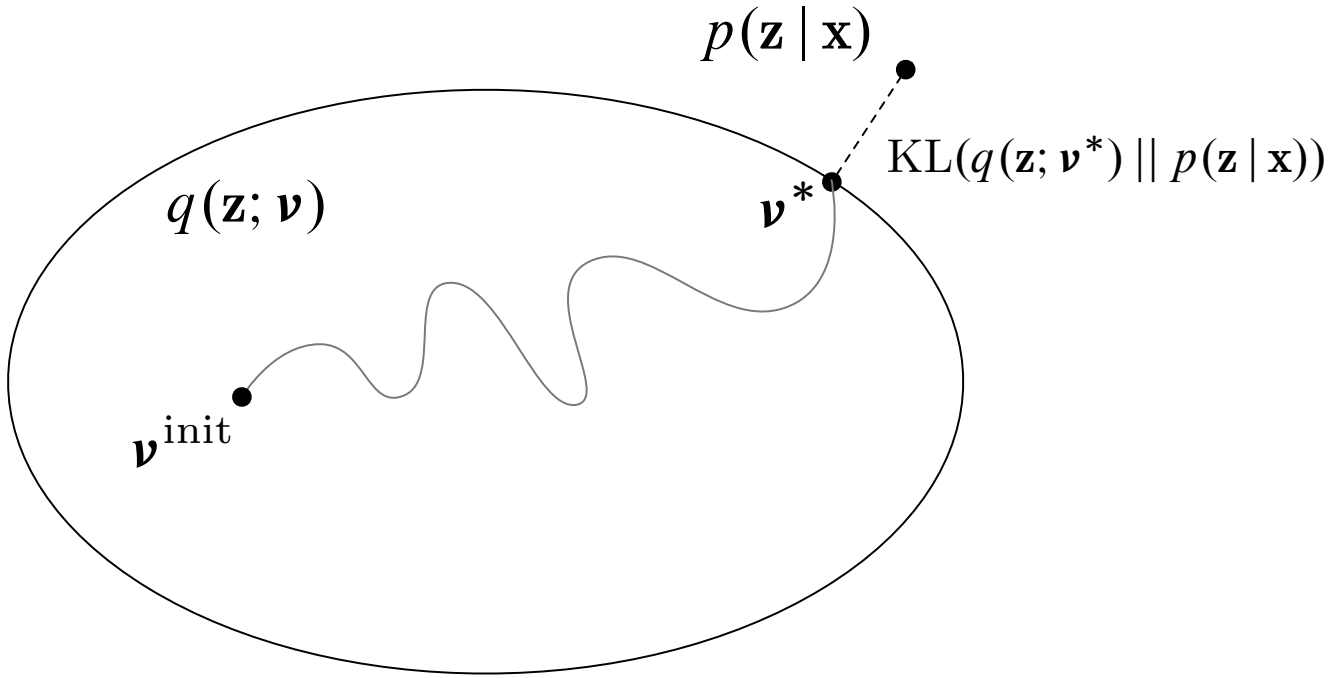


$$p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^{n} p(z_i, x_i \mid \beta)$$

- Bayesian mixture models
- Time series models
  (HMMs, linear dynamic systems)
- Factorial models
- Matrix factorization
  (factor analysis, PCA, CCA)
- Dirichlet process mixtures, HDPs
- Multilevel regression
  (linear, probit, Poisson)
- Stochastic block models
- Mixed-membership models
  (LDA and some variants)


all models
evaluable
conditionally
conjugate
differentiable

Variational inference



Minimize KL between $q(\beta, \mathbf{z}; \boldsymbol{\nu})$ and the posterior $p(\beta, \mathbf{z} \mid \mathbf{x})$.

The evidence lower bound

$$\mathcal{L}(\boldsymbol{\nu}) = \underbrace{\mathbb{E}_q\left[\log p(\beta, \mathbf{z}, \mathbf{x})\right]}_{\text{Expected complete log likelihood}} - \underbrace{\mathbb{E}_q\left[\log q(\beta, \mathbf{z}; \boldsymbol{\nu})\right]}_{\text{Negative entropy}}$$

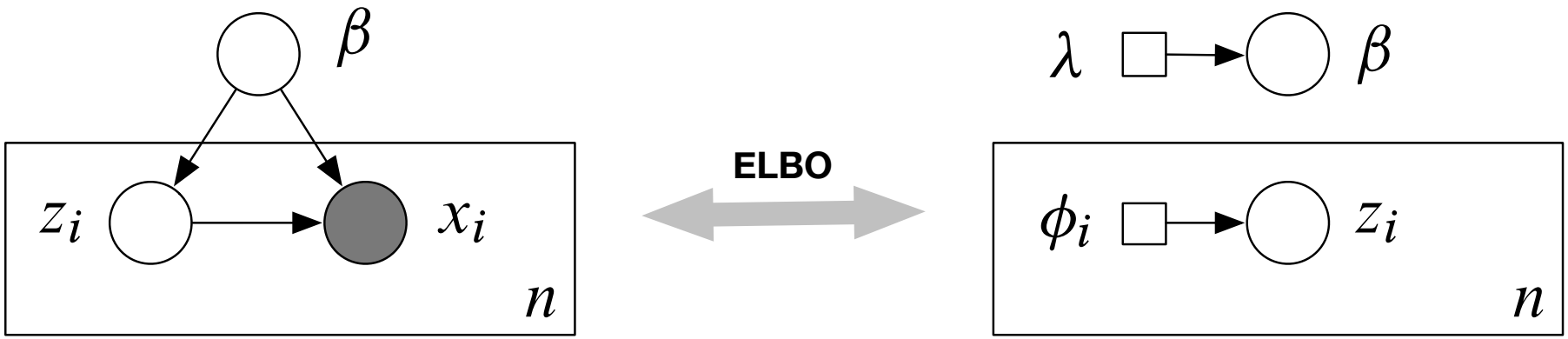
- KL is intractable; VI optimizes the **evidence lower bound** (ELBO) instead.
  - It is a lower bound on $\log p(\mathbf{x})$.
  - Maximizing the ELBO is equivalent to minimizing the KL.
- The ELBO trades off two terms.
  - The first term prefers $q(\cdot)$ to place its mass on the MAP estimate.
  - The second term encourages $q(\cdot)$ to be diffuse.
- Caveat: The ELBO is not convex.

The evidence lower bound

$$\mathcal{L}(\boldsymbol{\nu}) = \underbrace{\mathbb{E}_q\left[\log p(\mathbf{x} \mid \beta, \mathbf{z})\right]}_{\text{Expected log likelihood of data}} - \underbrace{\mathrm{KL}(q(\beta, \mathbf{z}; \boldsymbol{\nu}) \,||\, p(\beta, \mathbf{z}))}_{\text{KL between variational and prior}}$$

- KL is intractable; VI optimizes the **evidence lower bound** (ELBO) instead.
  - It is a lower bound on $\log p(\mathbf{x})$.
  - Maximizing the ELBO is equivalent to minimizing the KL.
- The ELBO trades off two terms.
  - The first term prefers $q(\cdot)$ to place its mass on the MLE.
  - The second term encourages $q(\cdot)$ to be close to the prior.
- Caveat: The ELBO is not convex.

Mean-field variational inference



- We need to specify the form of $q(\beta, \mathbf{z})$.
- The **mean-field family** is fully factorized,

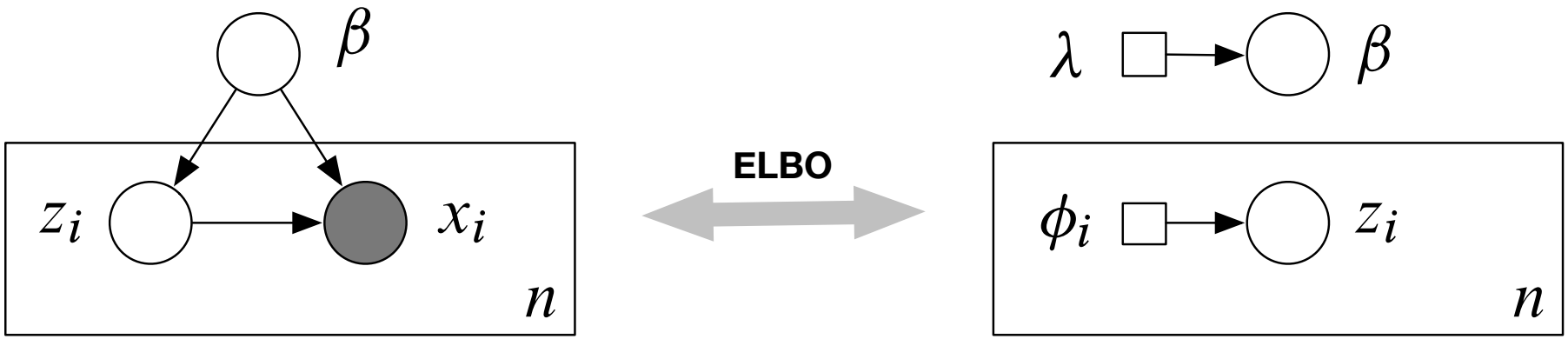
$$q(\beta, \mathbf{z}; \lambda, \boldsymbol{\phi}) = q(\beta; \lambda) \prod_{i=1}^{n} q(z_i; \phi_i).$$

- Each factor is the same family as the model's complete conditional,

$$p(\beta \mid \mathbf{z}, \mathbf{x}) = h(\beta) \exp\{\eta_g(\mathbf{z}, \mathbf{x})^\top \beta - a(\eta_g(\mathbf{z}, \mathbf{x}))\}$$
$$q(\beta; \lambda) = h(\beta) \exp\{\lambda^\top \beta - a(\lambda)\}.$$

(If the complete conditional is Gaussian then so is the variational factor.)

Mean-field variational inference



- Optimize the ELBO,

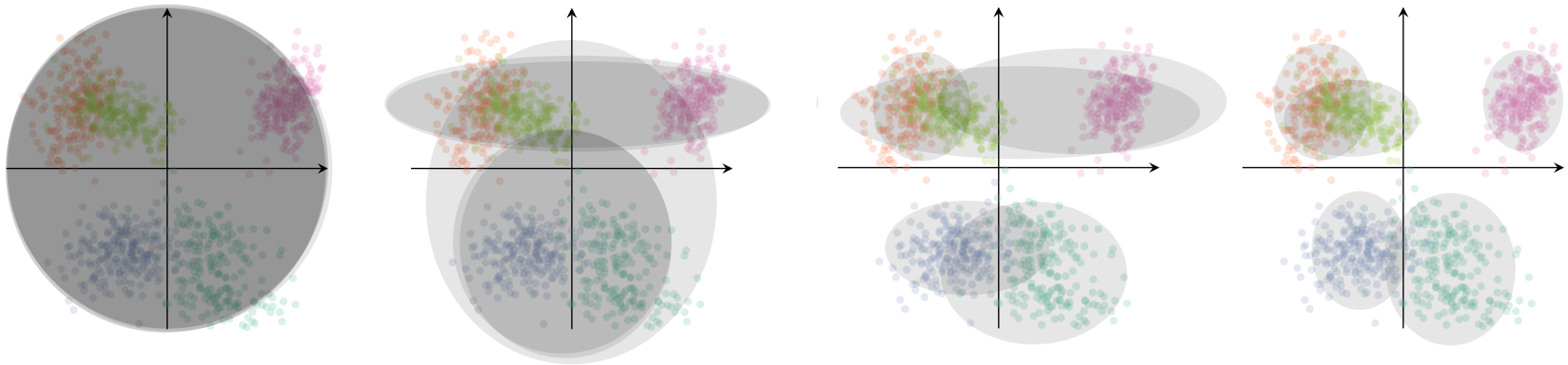
$$\mathcal{L}(\lambda, \boldsymbol{\phi}) = \mathbb{E}_q[\log p(\beta, \mathbf{z}, \mathbf{x})] - \mathbb{E}_q[\log q(\beta, \mathbf{z})].$$

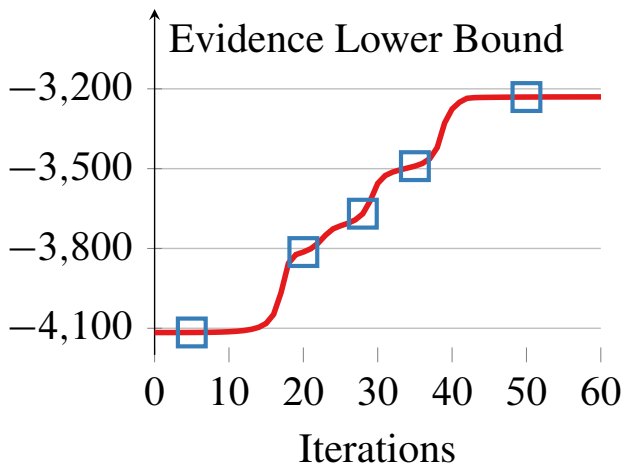
- Traditional VI uses coordinate ascent [Ghahramani and Beal, 2001]

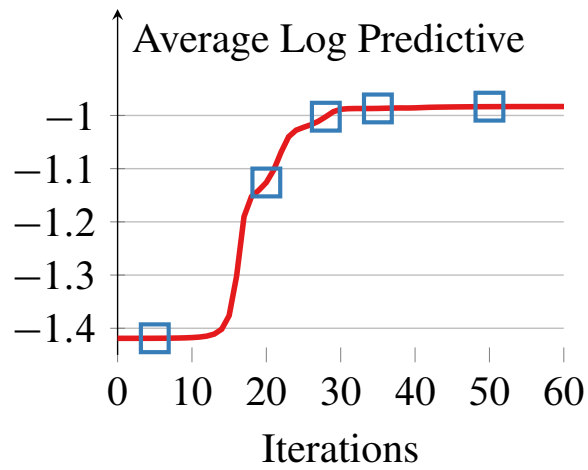
$$\lambda^* = \mathbb{E}_\phi\left[\eta_g(\mathbf{z}, \mathbf{x})\right];\ \phi_i^* = \mathbb{E}_\lambda\left[\eta_\ell(\beta, x_i)\right]$$

- Iteratively update each parameter, holding others fixed.
  - Notice the relationship to Gibbs sampling [Gelfand and Smith, 1990] .

Example: Mixture of Gaussians

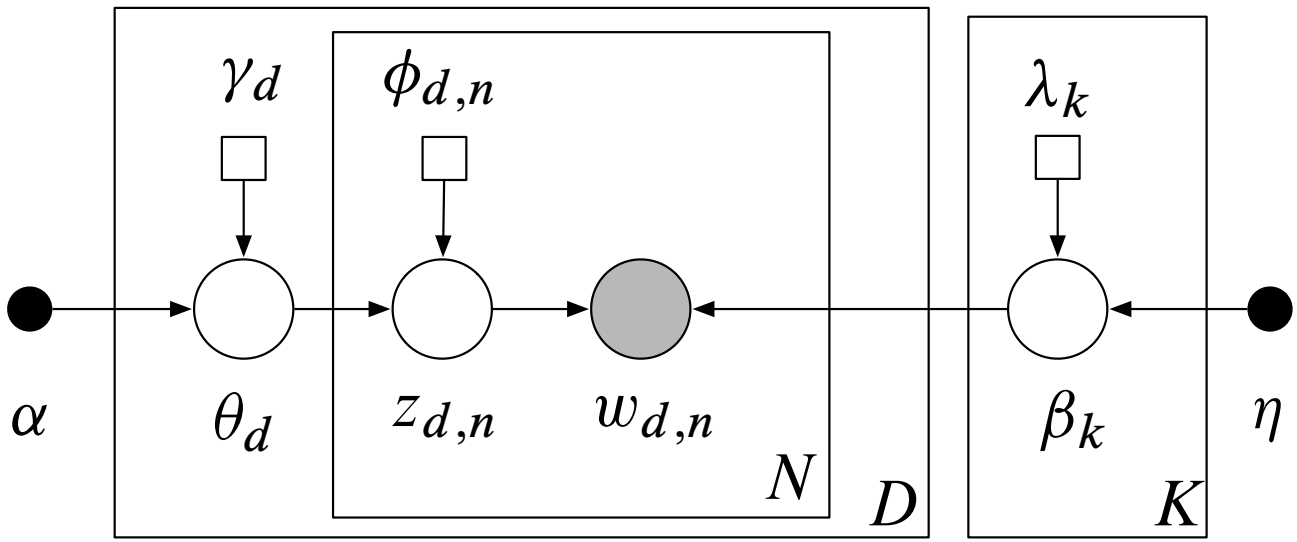






[images by Alp Kucukelbir; Blei+ 2016]

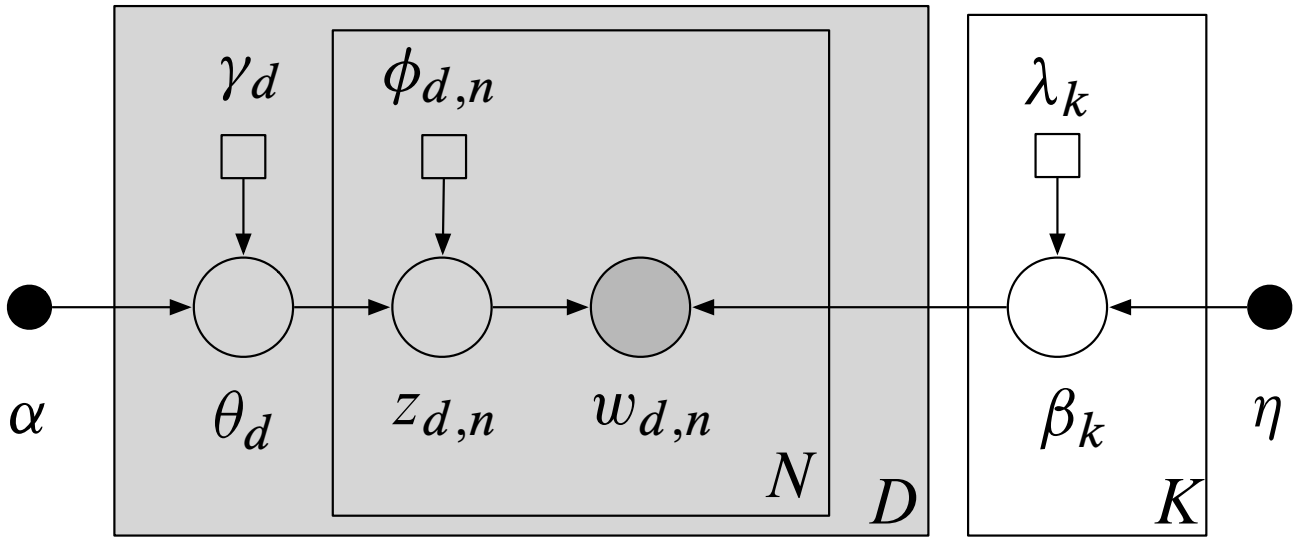
Mean-field variational inference for LDA



- The local variables are the per-document variables θ_d and $\mathbf{z}_d$.
- The global variables are the topics $\beta_1, \ldots, \beta_K$.
- The variational distribution is

$$q(\beta, \boldsymbol{\theta}, \mathbf{z}) = \prod_{k=1}^{K} q(\beta_k; \lambda_k) \prod_{d=1}^{D} q(\theta_d; \gamma_d) \prod_{n=1}^{N} q(z_{d,n}; \phi_{d,n})$$

Mean-field variational inference for LDA



- In the "local step" we iteratively update the parameters for each document, holding the topic parameters fixed.

$$\gamma^{(t+1)} = \alpha + \sum_{n=1}^{N} \phi_n^{(t)}$$

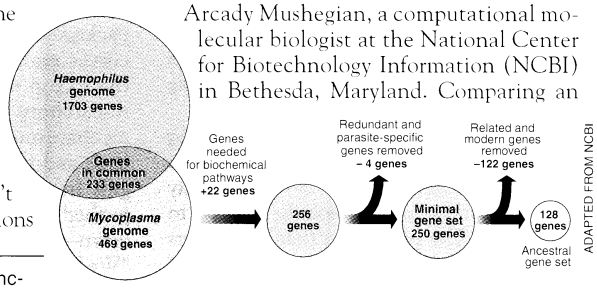
$$\phi_n^{(t+1)} \propto \exp\{\mathbb{E}[\log \theta] + \mathbb{E}[\log \beta_{\cdot,w_n}]\}.$$

Mean-field variational inference for LDA

Seeking Life's Bare (Genetic) Necessities

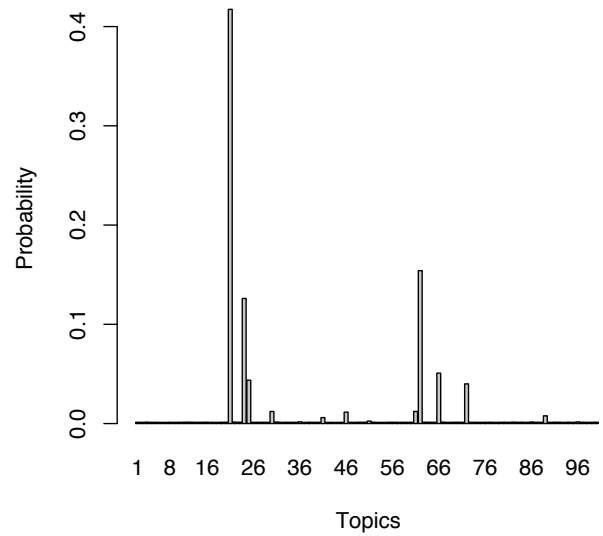
COLD SPRING HARBOR, NEW YORK—How many genes does an organism need to survive? Last week at the genome meeting here,* two genome researchers with radically different approaches presented complementary views of the basic genes needed for life. One research team, using computer analyses to compare known genomes, concluded that today's organisms can be sustained with just 250 genes, and that the earliest life forms required a mere 128 genes. The other researcher mapped genes in a simple parasite and estimated that for this organism, 800 genes are plenty to do the job—but that anything short of 100 wouldn't be enough.

Although the numbers don't match precisely, those predictions "are not all that far apart," especially in comparison to the 75,000 genes in the human genome, notes Siv Andersson of Uppsala University in Sweden, who arrived at the 800 number. But coming up with a consensus answer may be more than just a genetic numbers game, particularly as more and more genomes are completely mapped and sequenced. "It may be a way of organizing any newly sequenced genome," explains Arcady Mushegian, a computational molecular biologist at the National Center for Biotechnology Information (NCBI) in Bethesda, Maryland. Comparing an

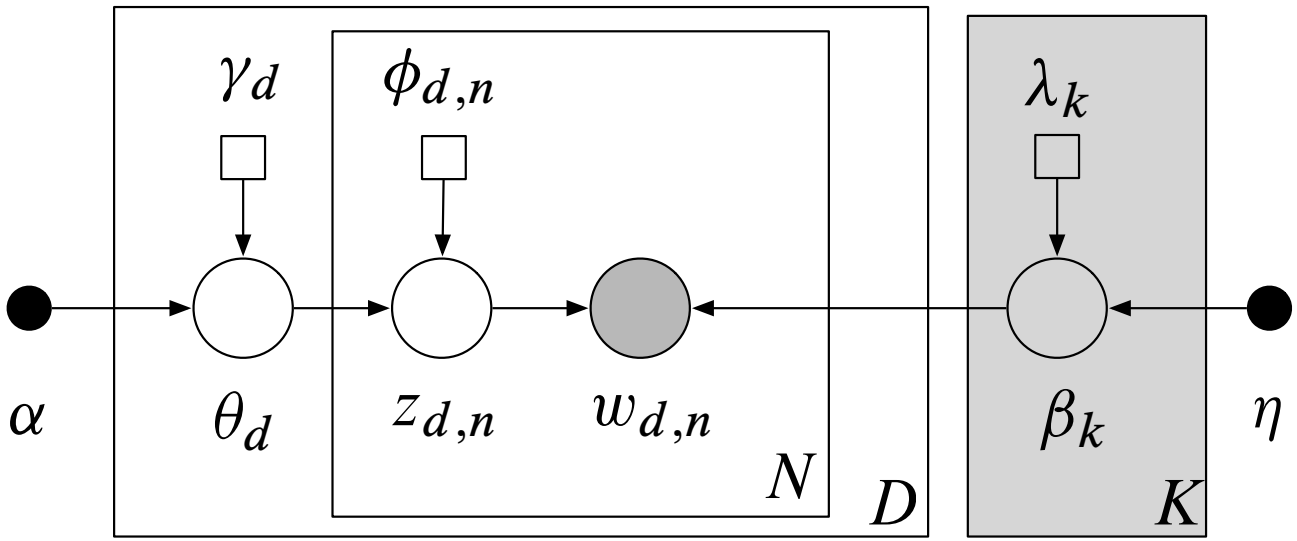


* Genome Mapping and Sequencing, Cold Spring Harbor, New York, May 8 to 12.

Stripping down. Computer analysis yields an estimate of the minimum modern and ancient genomes.



Mean-field variational inference for LDA



- In the "global step" we aggregate the parameters computed from the local step and update the parameters for the topics,

$$\lambda_k = \eta + \sum_d \sum_n w_{d,n} \phi_{d,n}.$$

Mean-field variational inference for LDA

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

Algorithm 1: Coordinate Ascent Variational Inference

Input: data $\mathbf{x}$, model $p(\beta, \mathbf{z}, \mathbf{x})$.

Initialize λ randomly.

while *not converged* **do**

  for *each data point* i **do**

    Set local parameter

$$\phi_i \leftarrow \mathbb{E}_\lambda \left[\eta_\ell(\beta, x_i) \right].$$

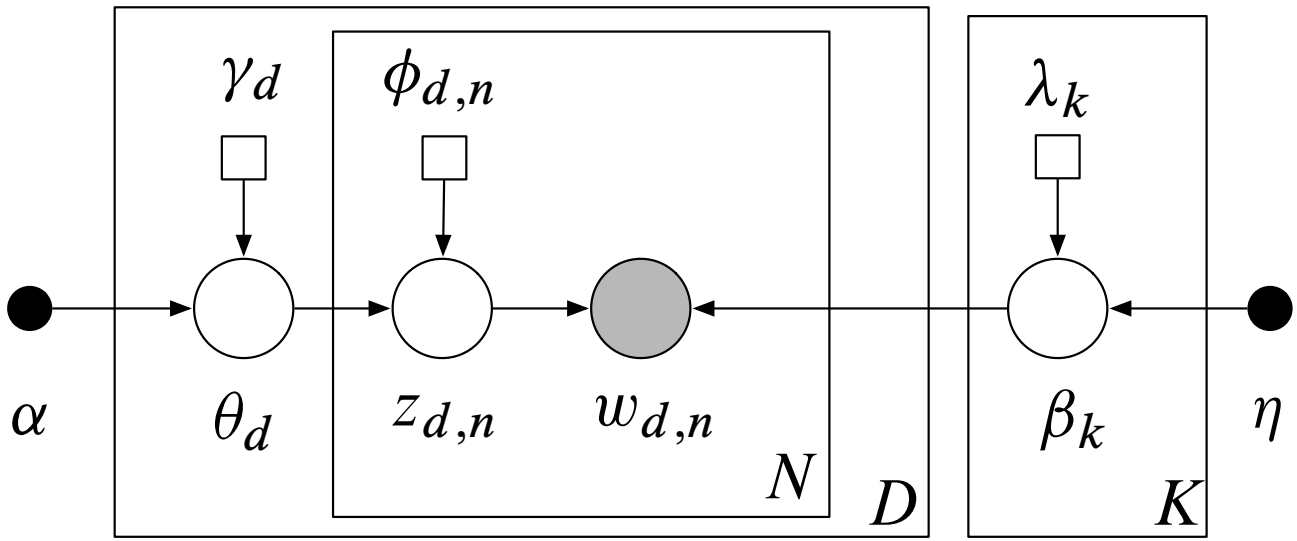
  end

  Set global parameter

$$\lambda \leftarrow \alpha + \sum_{i=1}^{n} \mathbb{E}_{\phi_i} \left[t(Z_i, x_i) \right].$$

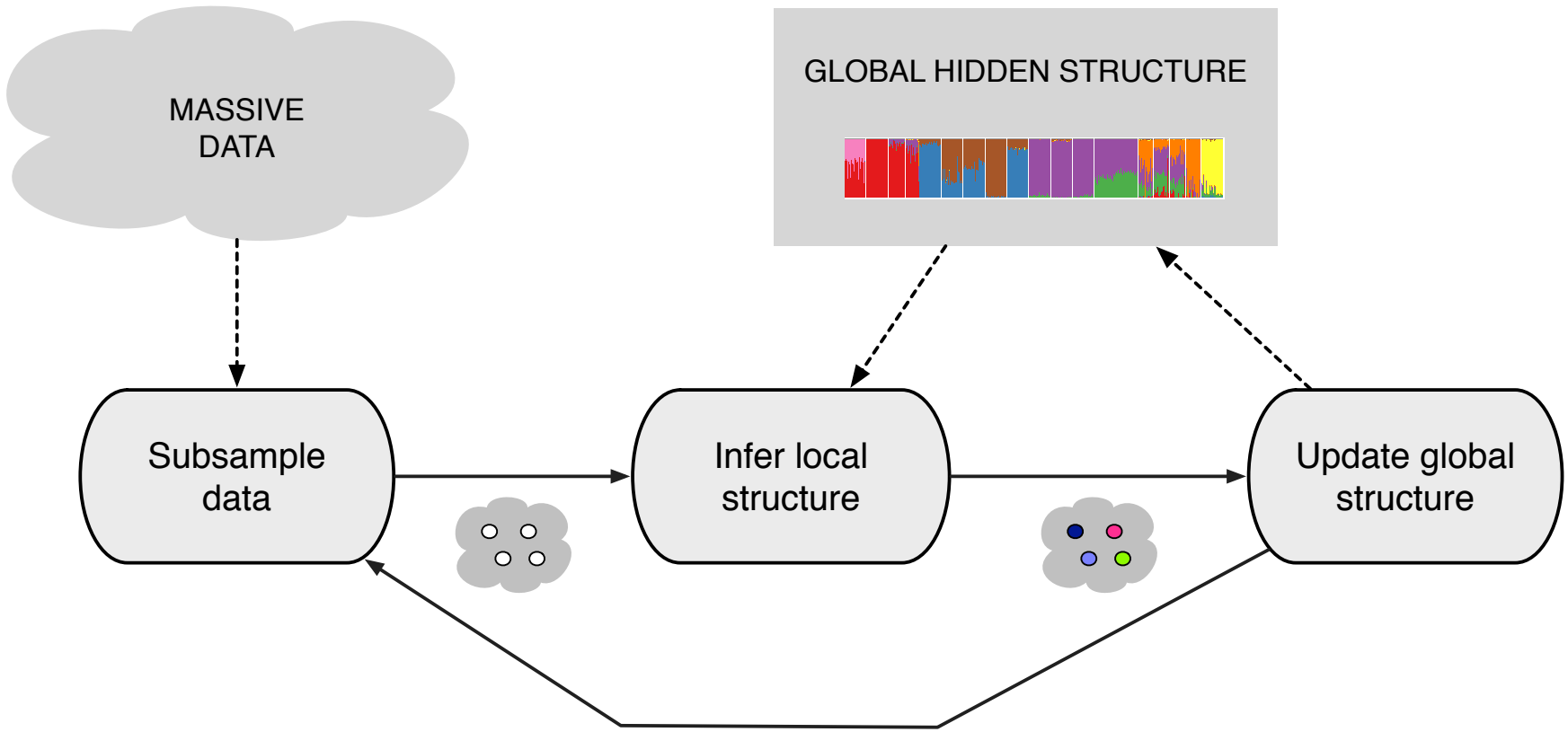
end

Stochastic variational inference



- Classical VI is inefficient:
  - Do some local computation *for each data point*.
  - Aggregate these computations to re-estimate global structure.
  - Repeat.
- This cannot handle massive data.
- **Stochastic variational inference** (SVI) scales VI to massive data.

Stochastic variational inference



Stochastic optimization

A STOCHASTIC APPROXIMATION METHOD[1]

By Herbert Robbins and Sutton Monro

University of North Carolina

1. Summary. Let $M(x)$ denote the expected value at level x of the response to a certain experiment. $M(x)$ is assumed to be a monotone function of x but is unknown to the experimenter, and it is desired to find the solution $x = \theta$ of the equation $M(x) = \alpha$, where α is a given constant. We give a method for making successive experiments at levels $x_1, x_2, \cdots$ in such a way that x_n will tend to θ in probability.

- Replace the gradient with cheaper noisy estimates [Robbins and Monro, 1951]
- Guaranteed to converge to a local optimum [Bottou, 1996]
- ***Has enabled modern machine learning***

Stochastic optimization

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- With noisy gradients, update

$$\nu_{t+1} = \nu_t + \rho_t \hat{\nabla}_\nu \mathscr{L}(\nu_t)$$

- Requires unbiased gradients, $\mathbb{E}\left[\hat{\nabla}_\nu \mathscr{L}(\nu)\right] = \nabla_\nu \mathscr{L}(\nu)$
- Requires the step size sequence ρ_t follows the Robbins-Monro conditions

Stochastic variational inference

- The **natural gradient** of the ELBO [Amari, 1998; Sato, 2001]

$$\nabla_\lambda^{\text{nat}} \mathcal{L}(\lambda) = \left(\alpha + \sum_{i=1}^n \mathbb{E}_{\phi_i^*}[t(Z_i, x_i)]\right) - \lambda.$$

- Construct a **noisy natural gradient**,

$$j \sim \text{Uniform}(1, \ldots, n)$$
$$\hat{\nabla}_\lambda^{\text{nat}} \mathcal{L}(\lambda) = \alpha + n\mathbb{E}_{\phi_j^*}[t(Z_j, x_j)] - \lambda.$$

- It is **good for stochastic optimization.**
  - Its expectation is the exact gradient (*unbiased*).
  - It only depends on optimized parameters of one data point (*cheap*).

Algorithm 2: Stochastic Variational Inference

Input: data $\mathbf{x}$, model $p(\beta, \mathbf{z}, \mathbf{x})$.

Initialize λ randomly.
Set ρ_t appropriately.

while *not converged* **do**

Sample $j \sim \text{Unif}(1, \ldots, n)$.
Set local parameter

$$\phi \leftarrow \mathbb{E}_\lambda \left[\eta_\ell(\beta, x_j) \right].$$

Set intermediate global parameter

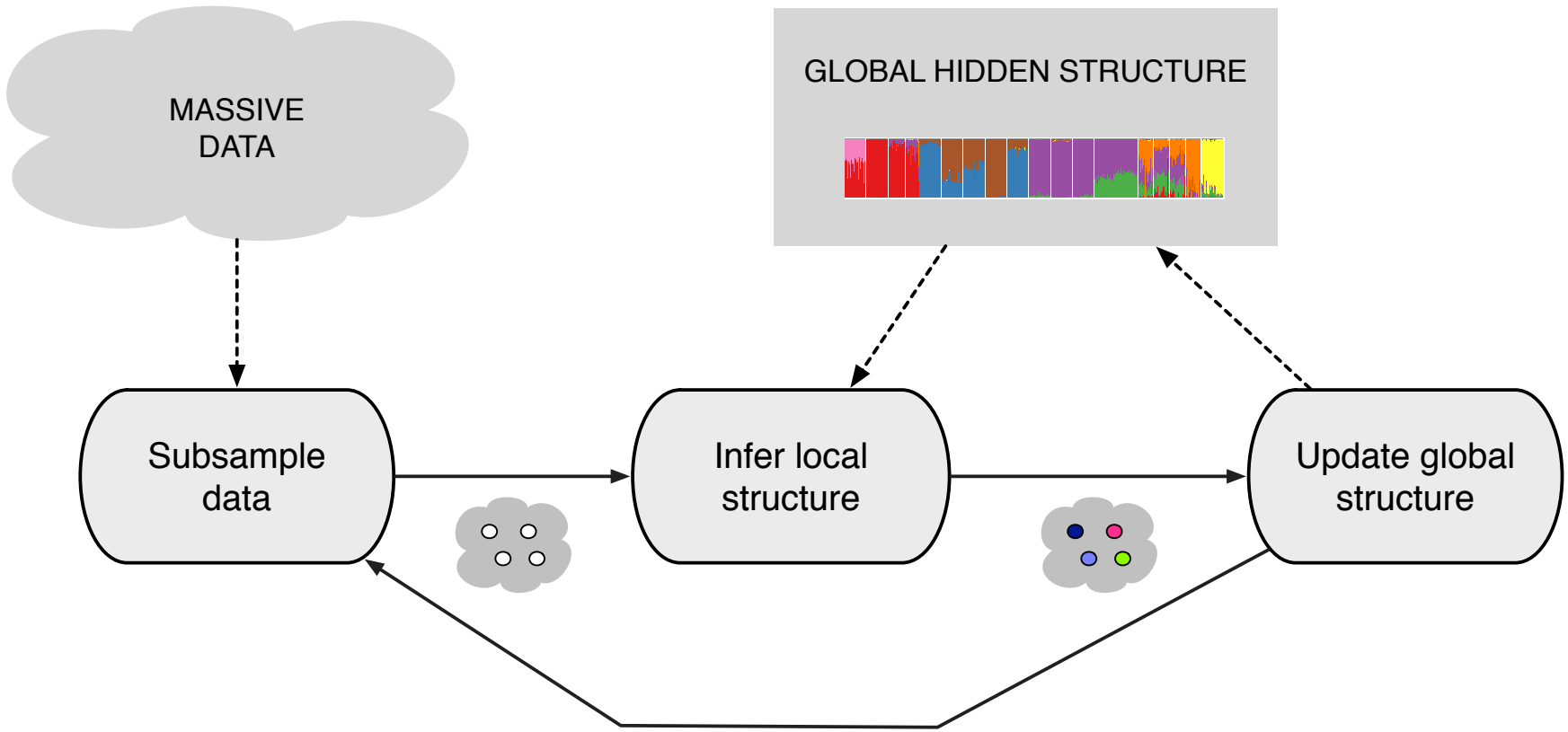
$$\hat{\lambda} = \alpha + n\mathbb{E}_\phi[t(Z_j, x_j)].$$

Set global parameter

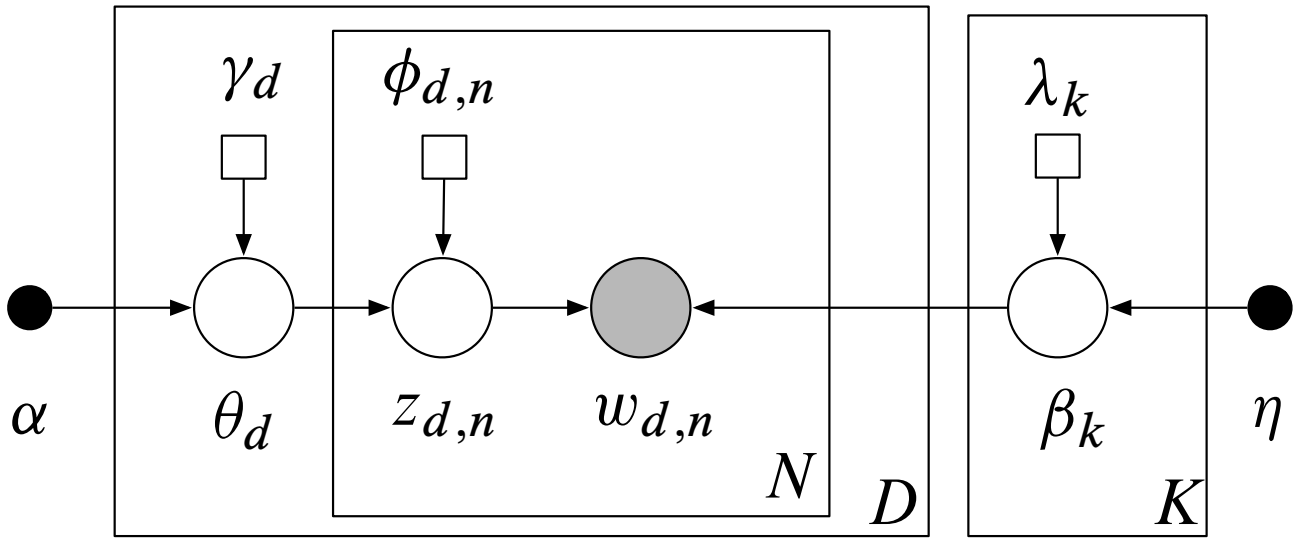
$$\lambda = (1 - \rho_t)\lambda + \rho_t \hat{\lambda}.$$

end

Stochastic variational inference

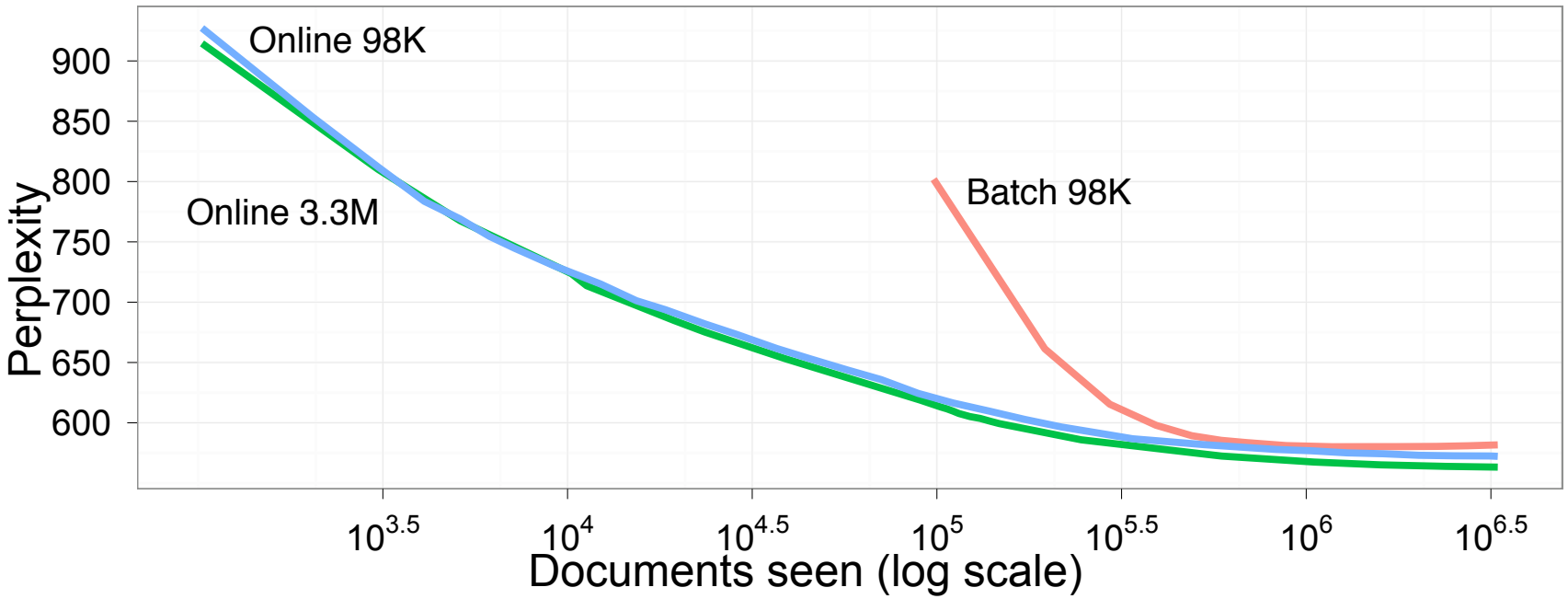


Stochastic variational inference for LDA



- Sample a document
- Estimate the local variational parameters using the current topics
- Form intermediate topics from those local parameters
- Update topics as a weighted average of intermediate and current topics

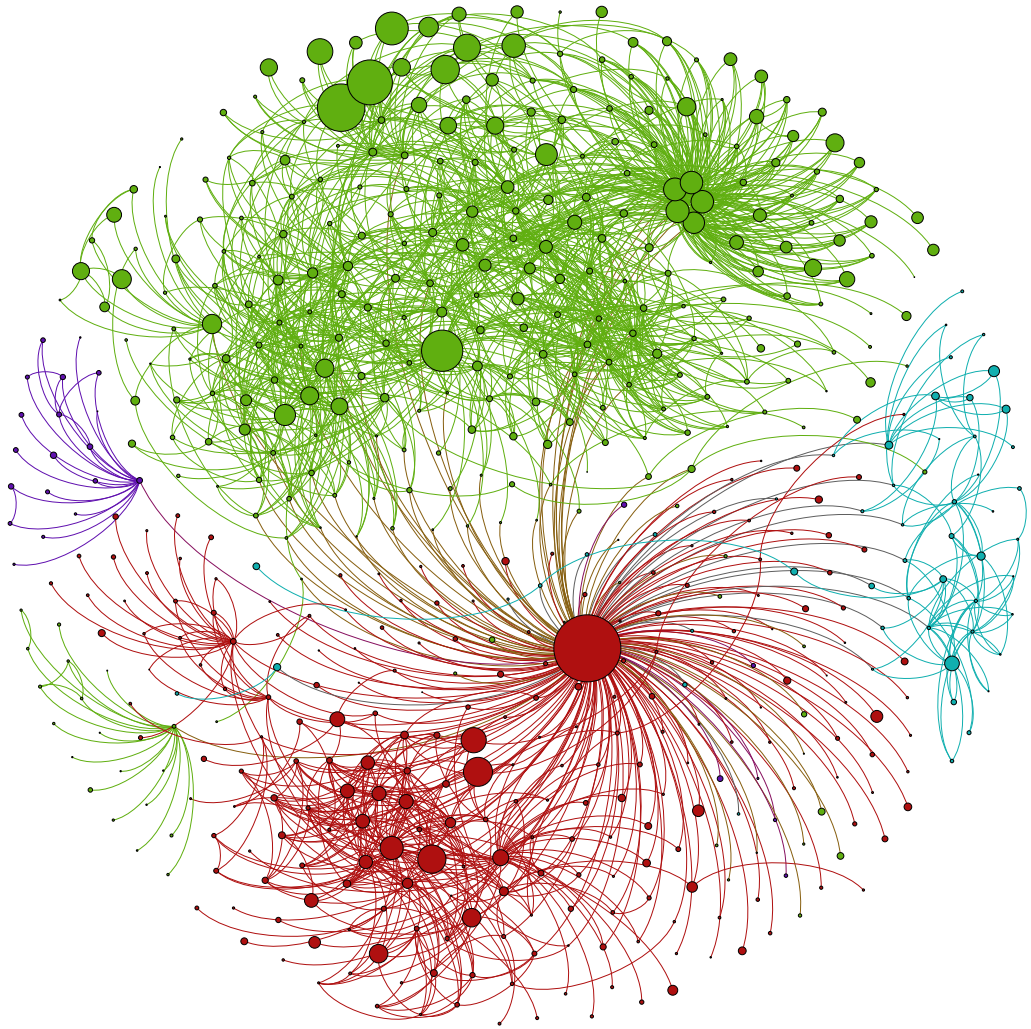
Stochastic variational inference for LDA



Documents analyzed	2048	4096	8192	12288	16384	32768	49152	65536
Top eight words	systems	systems	service	service	service	business	business	business
	road	health	systems	systems	companies	service	service	industry
	made	communication	health	companies	systems	companies	companies	service
	service	service	companies	business	business	industry	industry	companies
	announced	billion	market	company	company	company	services	services
	national	language	communication	billion	industry	management	company	company
	west	care	company	health	market	systems	management	management
	language	road	billion	industry	billion	services	public	public

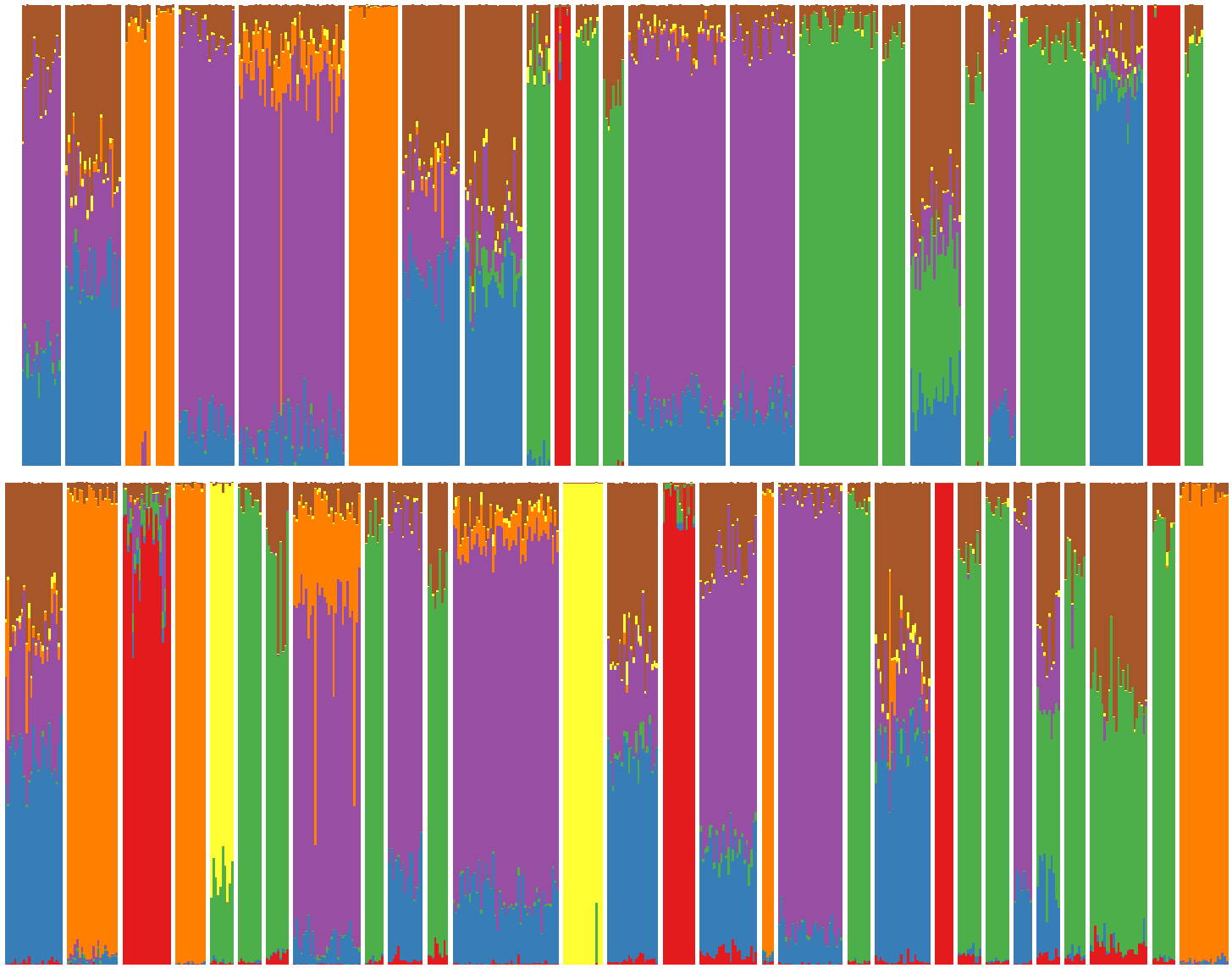
[Hoffman+ 2010]

Topics using the HDP, found in 1.8M articles from the New York Times



Communities discovered in a 3.7M node network of U.S. Patents

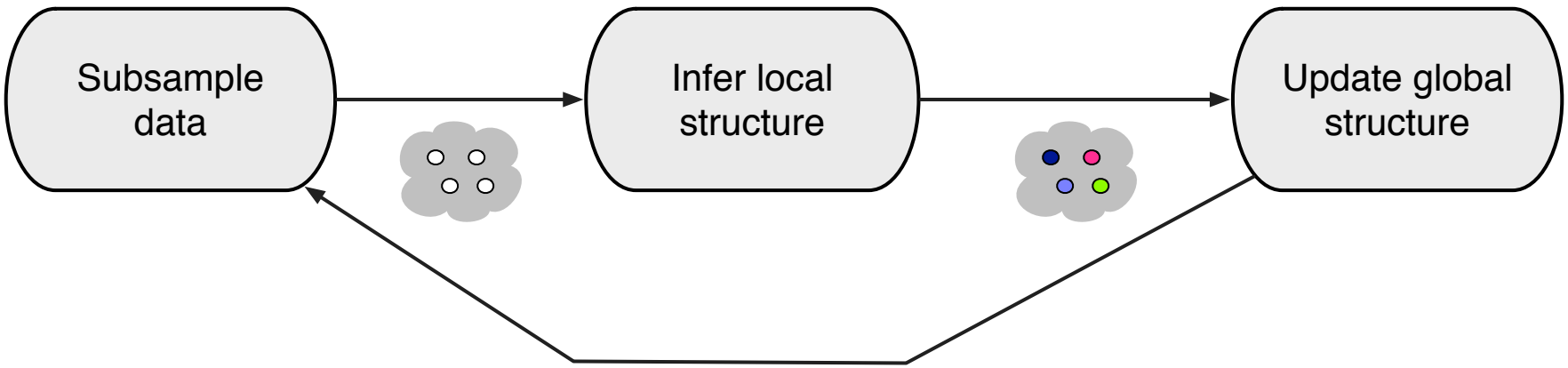
[Gopalan and Blei, PNAS 2013]



Population analysis of 2 billion genetic measurements

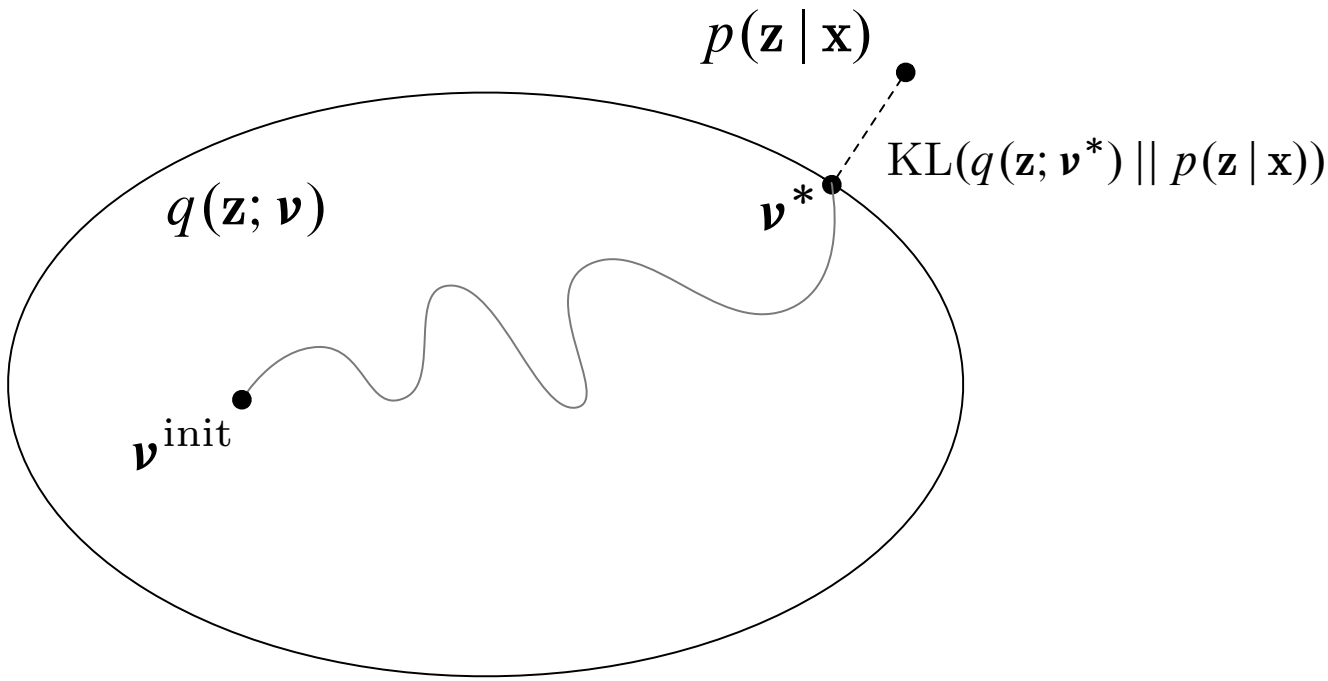
[Gopalan+ Nature Genetics 2016]

SVI scales many models



- Bayesian mixture models
- Time series models (HMMs, linear dynamic systems)
- Factorial models
- Matrix factorization (factor analysis, PCA, CCA)
- Dirichlet process mixtures, HDPs
- Multilevel regression (linear, probit, Poisson)
- Stochastic block models
- Mixed-membership models (LDA and some variants)

Variational inference



- VI solves **inference** with **optimization**.
- Posit a **variational family** of distributions over the latent variables.
- Fit the **variational parameters** $\boldsymbol{\nu}$ to be close (in KL) to the exact posterior.

A.1 Computing $\mathrm{E}[\log(\theta_i \mid \alpha)]$

The need to compute the expected value of the log of a single probability component under the Dirichlet arises repeatedly in deriving the inference and parameter estimation procedures for LDA. This value can be easily computed from the natural parameterization of the exponential family representation of the Dirichlet distribution.

Recall that a distribution is in the exponential family if it can be written in the form:

$$p(x \mid \eta) = h(x) \exp\left\{\eta^T T(x) - A(\eta)\right\},$$

where η is the natural parameter, $T(x)$ is the sufficient statistic, and $A(\eta)$ is the log of the normalization factor.

We can write the Dirichlet in this form by exponentiating the log of Eq. (1):

$$p(\theta \mid \alpha) = \exp\left\{\left(\sum_{i=1}^k (\alpha_i - 1)\log\theta_i\right) + \log\Gamma\left(\sum_{i=1}^k \alpha_i\right) - \sum_{i=1}^k \log\Gamma(\alpha_i)\right\}.$$

From this form, we immediately see that the natural parameter of the Dirichlet is $\eta_i = \alpha_i - 1$ and the sufficient statistic is $T(\theta_i) = \log\theta_i$. Furthermore, using the general fact that the derivative of the log normalization factor with respect to the natural parameter is equal to the expectation of the sufficient statistic, we obtain:

$$\mathrm{E}[\log\theta_i \mid \alpha] = \Psi(\alpha_i) - \Psi\left(\sum_{j=1}^k \alpha_j\right)$$

where Ψ is the digamma function, the first derivative of the log Gamma function.

A.3.2 Variational Dirichlet

Next, we maximize Eq. (15) with respect to γ_i, the ith component of the posterior Dirichlet parameter. The terms containing γ_i are:

$$\begin{aligned} L_{[\gamma]} = &\sum_{i=1}^k (\alpha_i - 1)\left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right) + \sum_{n=1}^N \phi_{ni}\left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right) \\ &- \log\Gamma\left(\sum_{j=1}^k \gamma_j\right) + \log\Gamma(\gamma_i) - \sum_{i=1}^k (\gamma_i - 1)\left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right). \end{aligned}$$

This simplifies to:

$$L_{[\gamma]} = \sum_{i=1}^k \left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right)\left(\alpha_i + \sum_{n=1}^N \phi_{ni} - \gamma_i\right) - \log\Gamma\left(\sum_{j=1}^k \gamma_j\right) + \log\Gamma(\gamma_i).$$

We take the derivative with respect to γ_i:

$$\frac{\partial L}{\partial \gamma_i} = \Psi'(\gamma_i)\left(\alpha_i + \sum_{n=1}^N \phi_{ni} - \gamma_i\right) - \Psi'\left(\sum_{j=1}^k \gamma_j\right)\sum_{j=1}^k \left(\alpha_j + \sum_{n=1}^N \phi_{nj} - \gamma_j\right).$$

Setting this equation to zero yields a maximum at:

$$\gamma_i = \alpha_i + \sum_{n=1}^N \phi_{ni}. \tag{17}$$

Since Eq. (17) depends on the variational multinomial ϕ, full variational inference requires alternating between Eqs. (16) and (17) until the bound converges.

Finally, we expand Eq. (14) in terms of the model parameters (α, β) and the variational parameters (γ, ϕ). Each of the five lines below expands one of the five terms in the bound:

$$\begin{aligned} L(\gamma, \phi; \alpha, \beta) = &\log\Gamma\left(\sum_{j=1}^k \alpha_j\right) - \sum_{i=1}^k \log\Gamma(\alpha_i) + \sum_{i=1}^k (\alpha_i - 1)\left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right) \\ &+ \sum_{n=1}^N \sum_{i=1}^k \phi_{ni}\left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right) \\ &+ \sum_{n=1}^N \sum_{i=1}^k \sum_{j=1}^V \phi_{ni} w_n^j \log\beta_{ij} \\ &- \log\Gamma\left(\sum_{j=1}^k \gamma_j\right) + \sum_{i=1}^k \log\Gamma(\gamma_i) - \sum_{i=1}^k (\gamma_i - 1)\left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right) \\ &- \sum_{n=1}^N \sum_{i=1}^k \phi_{ni}\log\phi_{ni}, \end{aligned} \tag{15}$$

where we have made use of Eq. (8).

In the following two sections, we show how to maximize this lower bound with respect to the variational parameters ϕ and γ.

A.3.1 Variational multinomial

We first maximize Eq. (15) with respect to ϕ_{ni}, the probability that the nth word is generated by latent topic i. Observe that this is a constrained maximization since $\sum_{i=1}^k \phi_{ni} = 1$.

We form the Lagrangian by isolating the terms which contain ϕ_{ni} and adding the appropriate Lagrange multipliers. Let β_{iv} be $p(w_n^v = 1 \mid z^i = 1)$ for the appropriate v. (Recall that each w_n is a vector of size V with exactly one component equal to one; we can select the unique v such that $w_n^v = 1$):

$$L_{[\phi_{ni}]} = \phi_{ni}\left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right) + \phi_{ni}\log\beta_{iv} - \phi_{ni}\log\phi_{ni} + \lambda_n\left(\sum_{j=1}^k \phi_{ni} - 1\right),$$

where we have dropped the arguments of L for simplicity, and where the subscript ϕ_{ni} denotes that we have retained only those terms in L that are a function of ϕ_{ni}. Taking derivatives with respect to ϕ_{ni}, we obtain:

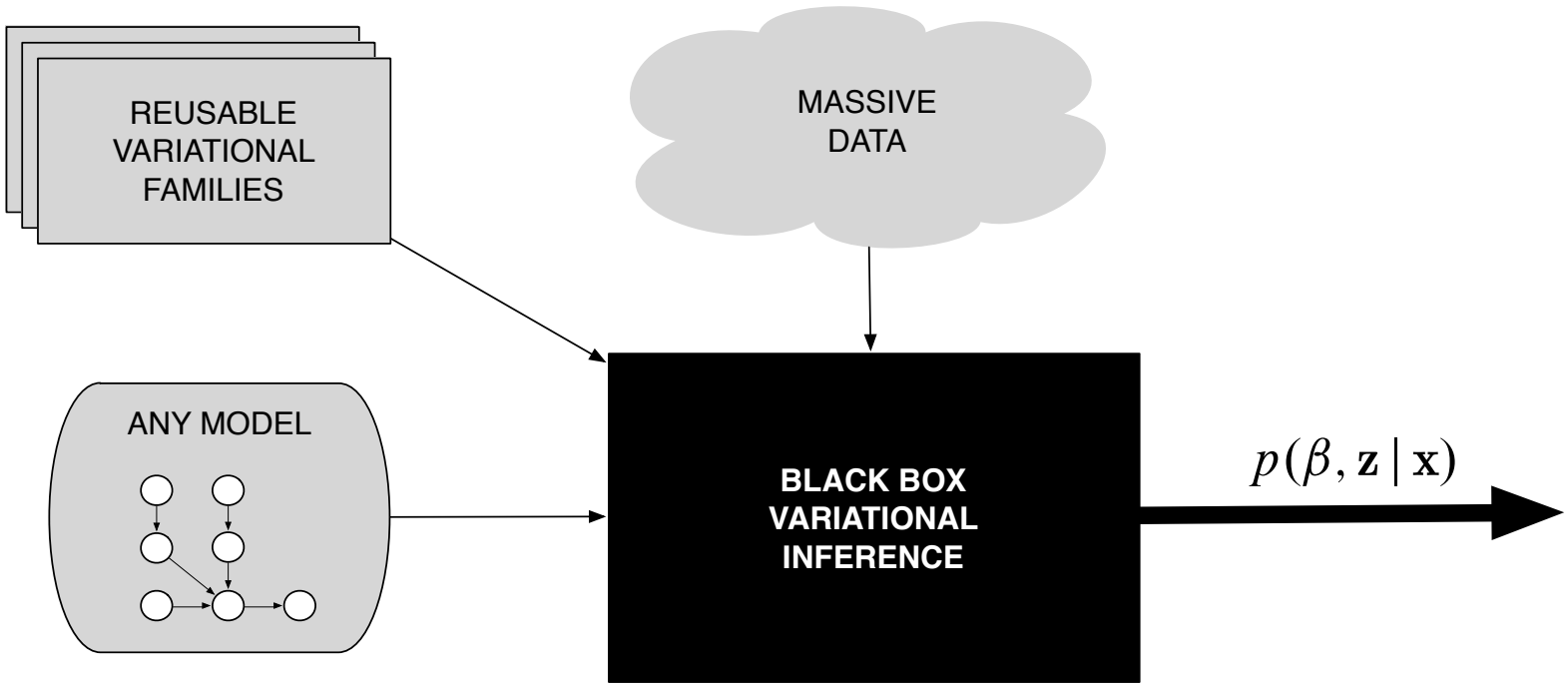
$$\frac{\partial L}{\partial \phi_{ni}} = \Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right) + \log\beta_{iv} - \log\phi_{ni} - 1 + \lambda.$$

Setting this derivative to zero yields the maximizing value of the variational parameter ϕ_{ni} (cf. Eq. 6):

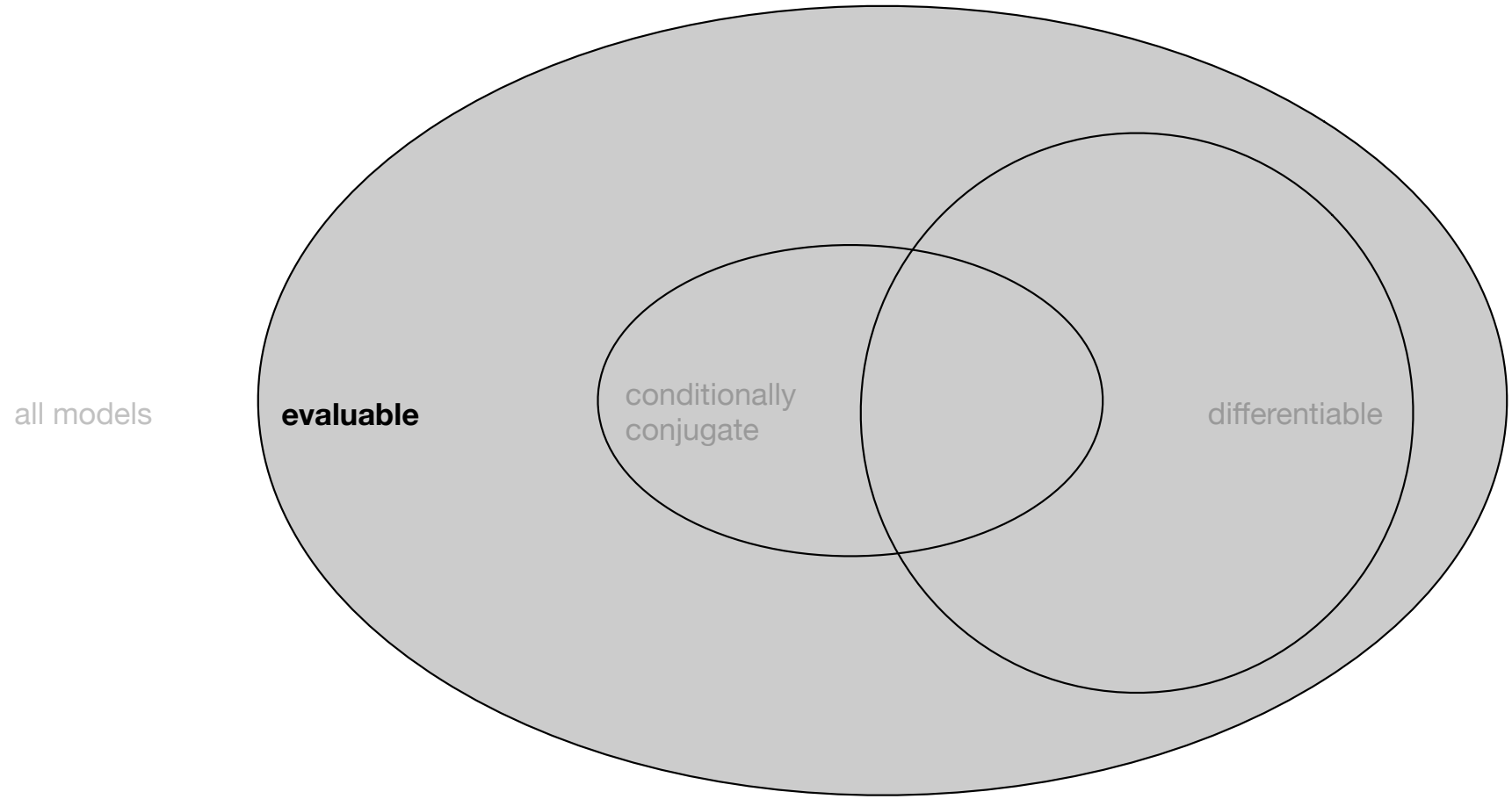
$$\phi_{ni} \propto \beta_{iv}\exp\left(\Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right)\right). \tag{16}$$

[from Blei+ 2003]

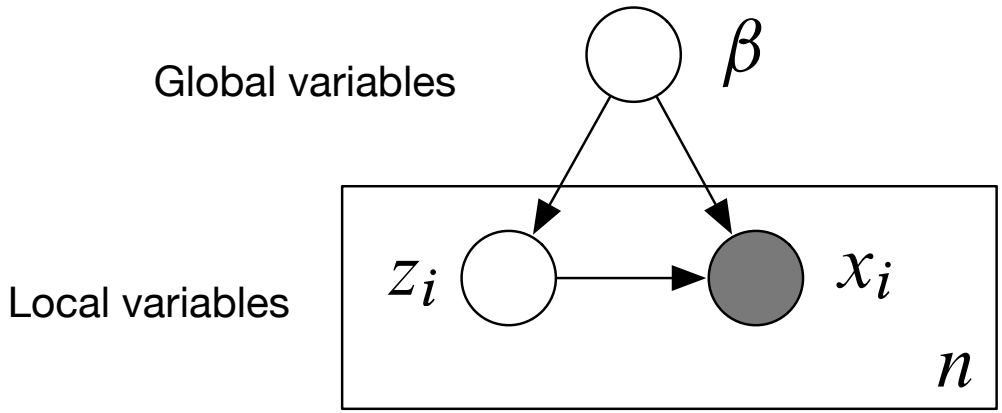
Black box variational inference



- Easily use variational inference with **any model**
- Perform inference with **massive data**
- **No mathematical work** beyond specifying the model


all models
evaluable
conditionally
conjugate
differentiable

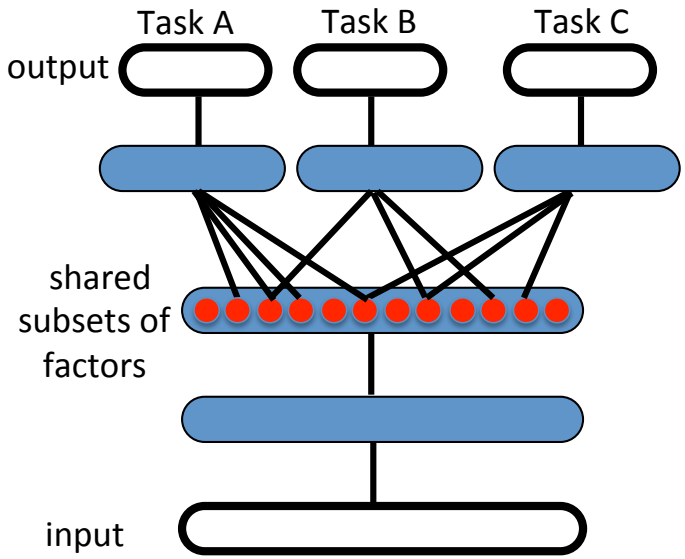
Nonconjugate models

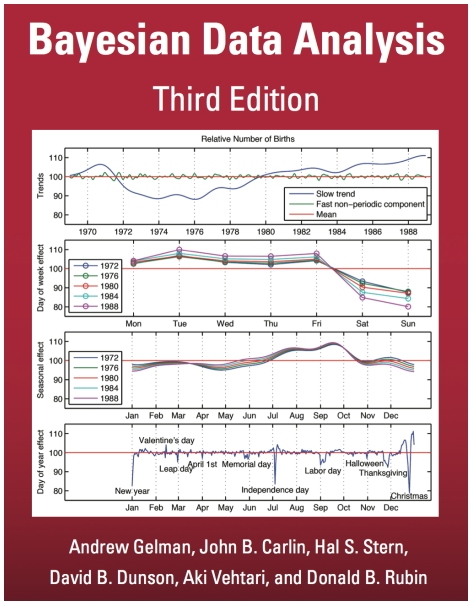


$$p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^{n} p(z_i, x_i \mid \beta)$$

- Nonlinear time series models
- Deep latent Gaussian models
- Models with attention
- Generalized linear models
- Stochastic volatility models
- Discrete choice models
- Bayesian neural networks
- Deep exponential families
- Correlated topic models
- Sigmoid belief networks

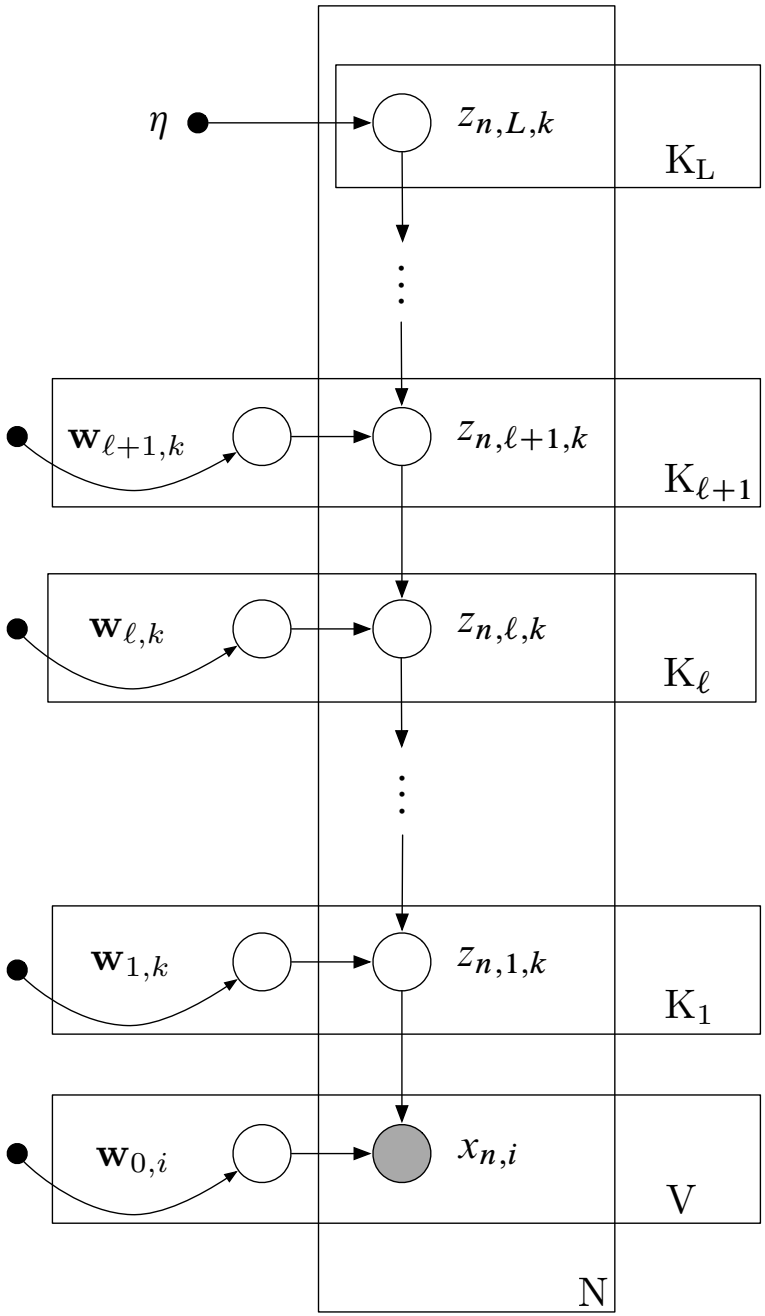
Deep exponential families (a digression)





- *Deep learning* [Bengio+ 2013]
  Discover layered representations of high-dimensional data.
- *Bayesian statistics* [Gelman+ 2014]
  Cast inferences of unknown quantities as probability calculations.
- *Bayesian deep learning* [Ranganath+ 2015]
  Posterior inference of layered representations of high-dimensional data.

Deep exponential families

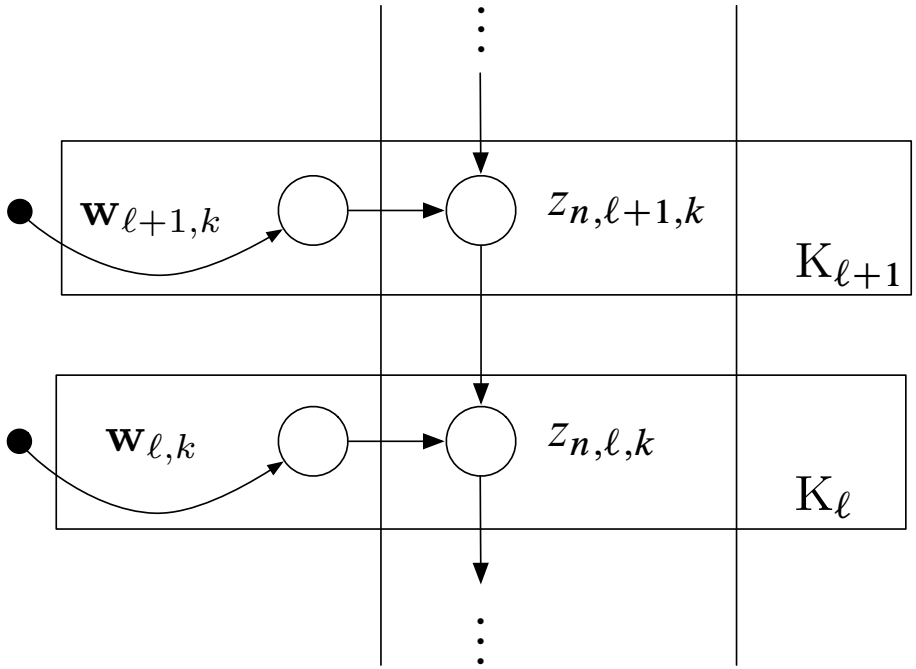


$z_{n,L,k} \sim \text{Exp-Fam}(\eta)$

$z_{n,\ell,k} \sim \text{Exp-Fam}(g(\mathbf{w}_{\ell,k}^\top \mathbf{z}_{n,\ell+1}))$

$x_{n,i} \sim \text{Exp-Fam}(g(\mathbf{w}_{0,i}^\top \mathbf{z}_{n,1}))$

Deep exponential families



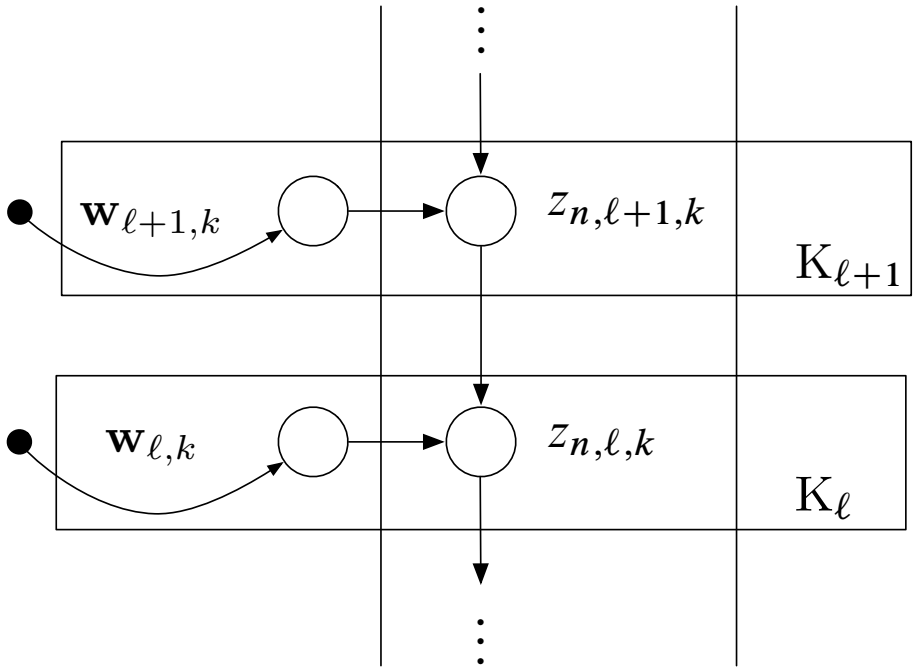
$$z_{n,\ell,k} \sim \text{Exp-Fam}(g(\mathbf{w}_{\ell,k}^\top \mathbf{z}_{n,\ell+1}))$$

- All distributions are in canonical exponential family form

$$p(z_{n,\ell,k} \mid \mathbf{z}_{n,\ell+1}, \mathbf{w}_{\ell,k}) = \exp\{\eta(\cdot)^\top t(z_{n,\ell,k}) - a(\eta(\cdot))\}.$$

- The natural parameter uses a link function, $\eta(\cdot) = g(\mathbf{z}_{n,\ell+1}^\top \mathbf{w}_{\ell,k})$.
- DEF design choices:
  - number of layers; number of units per layer
  - type of representation; link function

Deep exponential families

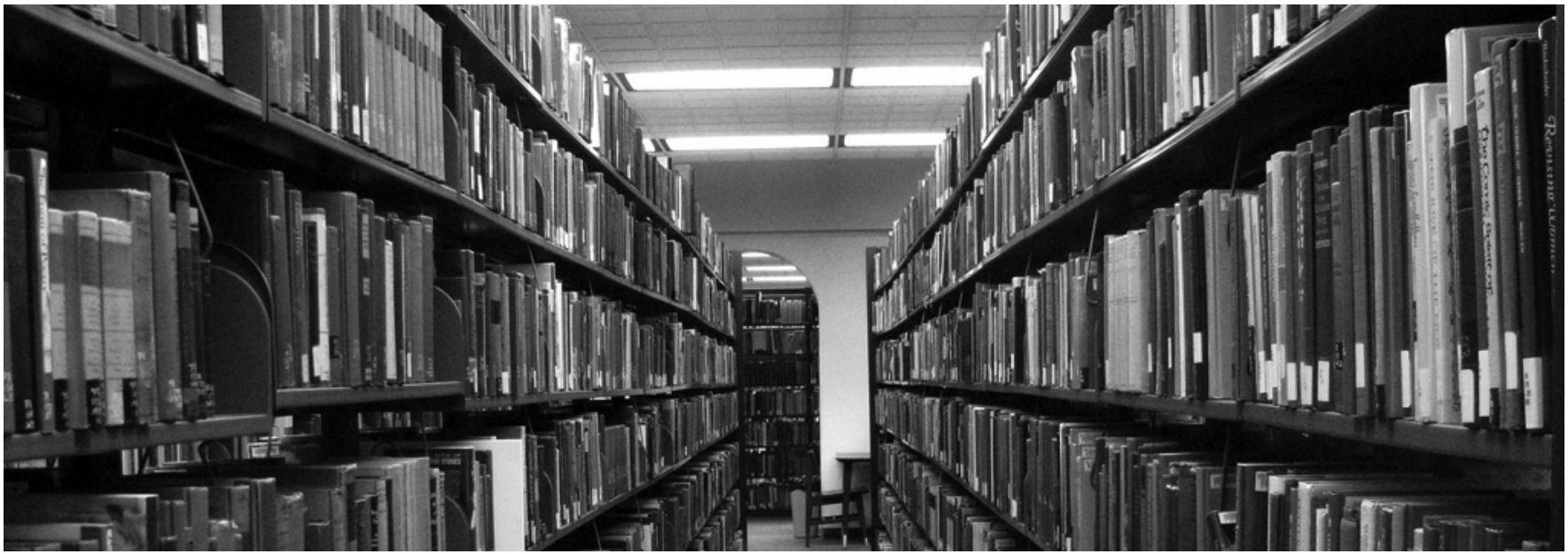


$$z_{n,\ell,k} \sim \textsc{Exp-Fam}(g(\mathbf{w}_{\ell,k}^\top \mathbf{z}_{n,\ell+1}))$$

The hidden layers:

- *Bernoulli*, for binary representations [Sigmoid Belief Net, Neal 1992]
- *Poisson*, for count representations
- *Gaussian*, for real representations
- *Gamma*, for positive representations

Example: Text data

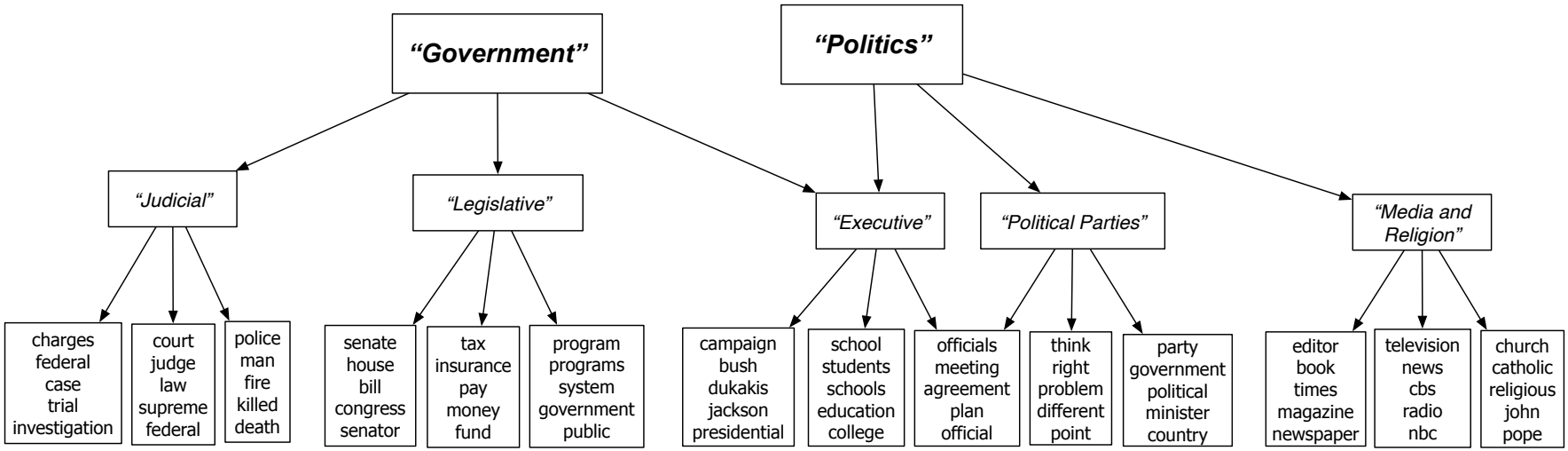


- In discrete data, $x_{n,i}$ is a count, e.g. of word i in document n
- At the bottom, use a Poisson likelihood

$$x_{n,i} \sim \text{Poisson}(g(\mathbf{w}_{0,i}^\top \mathbf{z}_{n,1}))$$

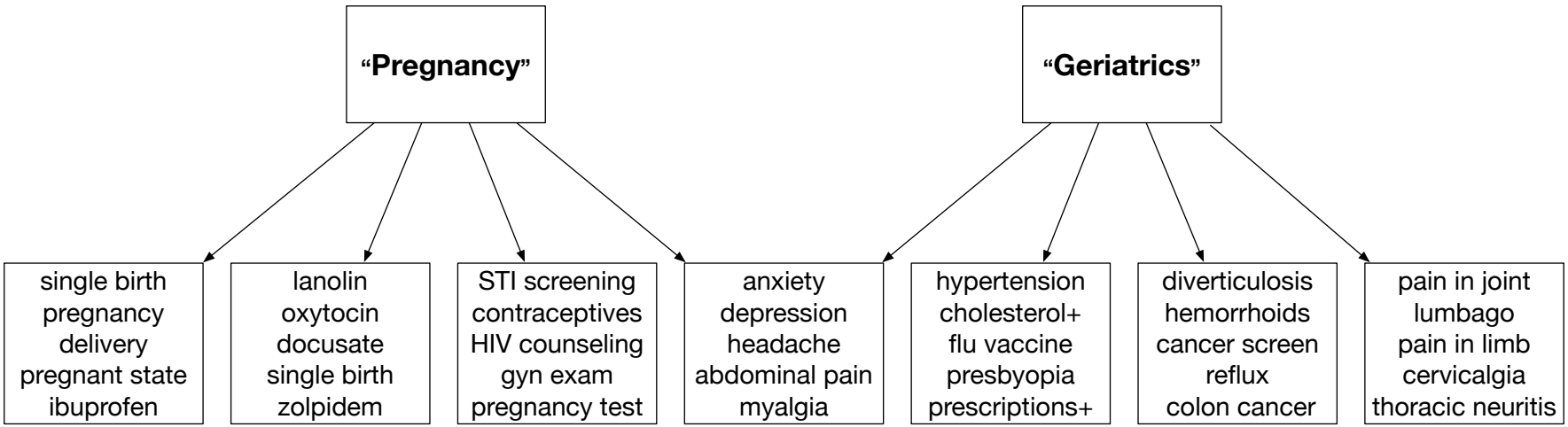
- This is an alternative to LDA that finds layers of topics

New York Times



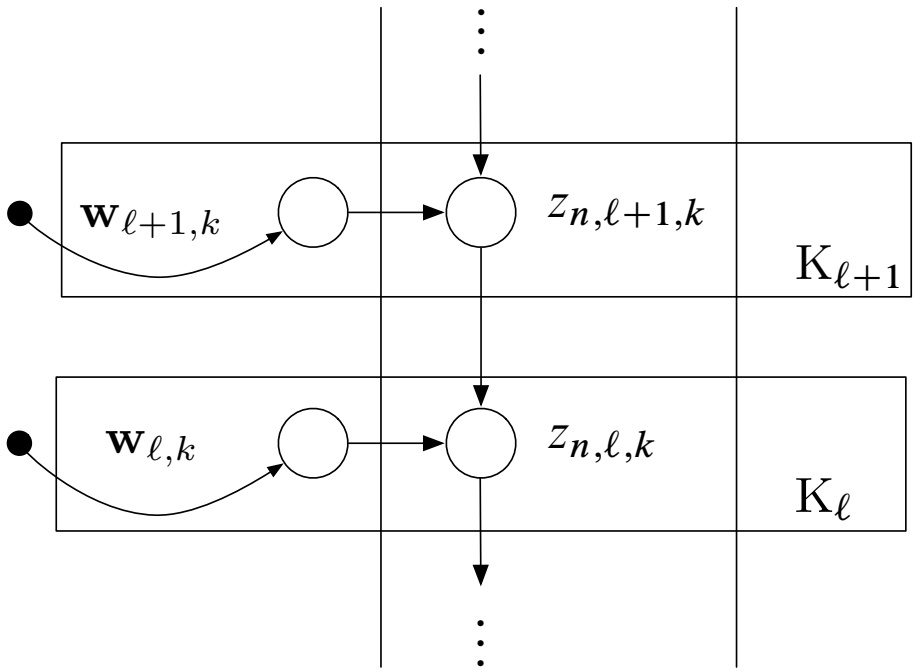
- 160,000 documents
- 8,500 vocabulary terms
- 10M observed words

Medical Diagnoses



- 300,000 patients
- 18,000 diagnoses and medicines
- 1.5M observed diagnoses

Deep exponential families

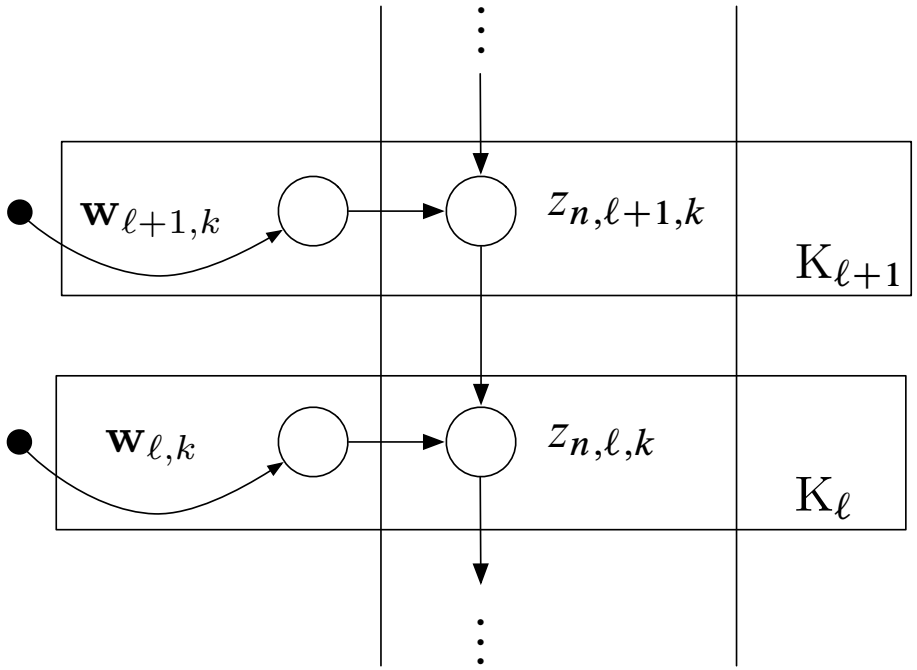


$$z_{n,\ell,k} \sim \textsc{Exp-Fam}(g(\mathbf{w}_{\ell,k}^\top \mathbf{z}_{n,\ell+1}))$$

- DEFs can be composed in more complex models
  - Text analysis
  - Collaborative filtering ("double DEFs")
  - Survival analysis
- Open source software:

`https://github.com/blei-lab/deep-exponential-families`

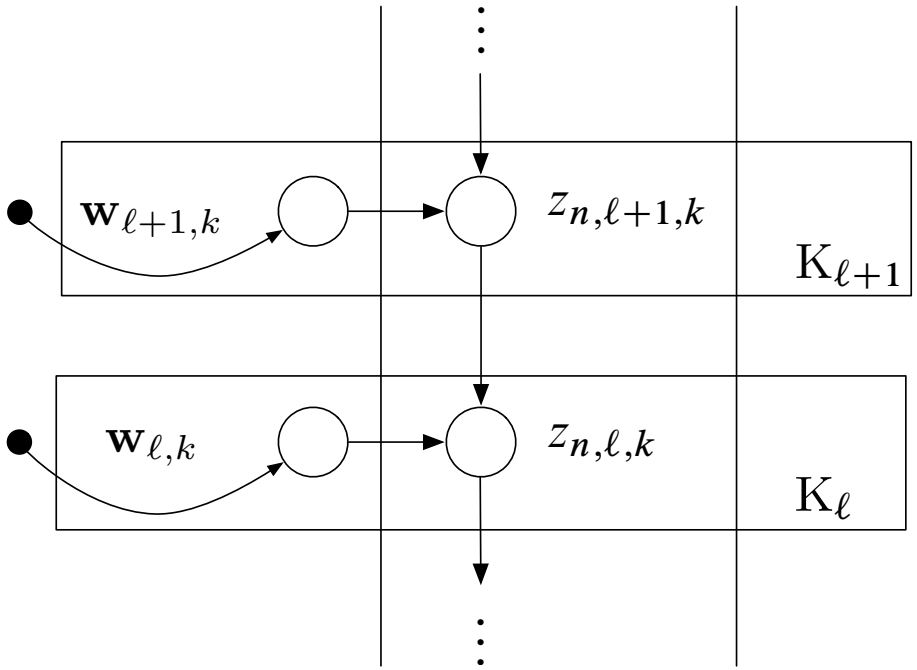
Deep exponential families



$$z_{n,\ell,k} \sim \textsc{Exp-Fam}(g(\mathbf{w}_{\ell,k}^\top \mathbf{z}_{n,\ell+1}))$$

- How to do inference?
- DEFs are *not* in the class of conditionally conjugate models.
- The complete conditionals do not have a closed form.

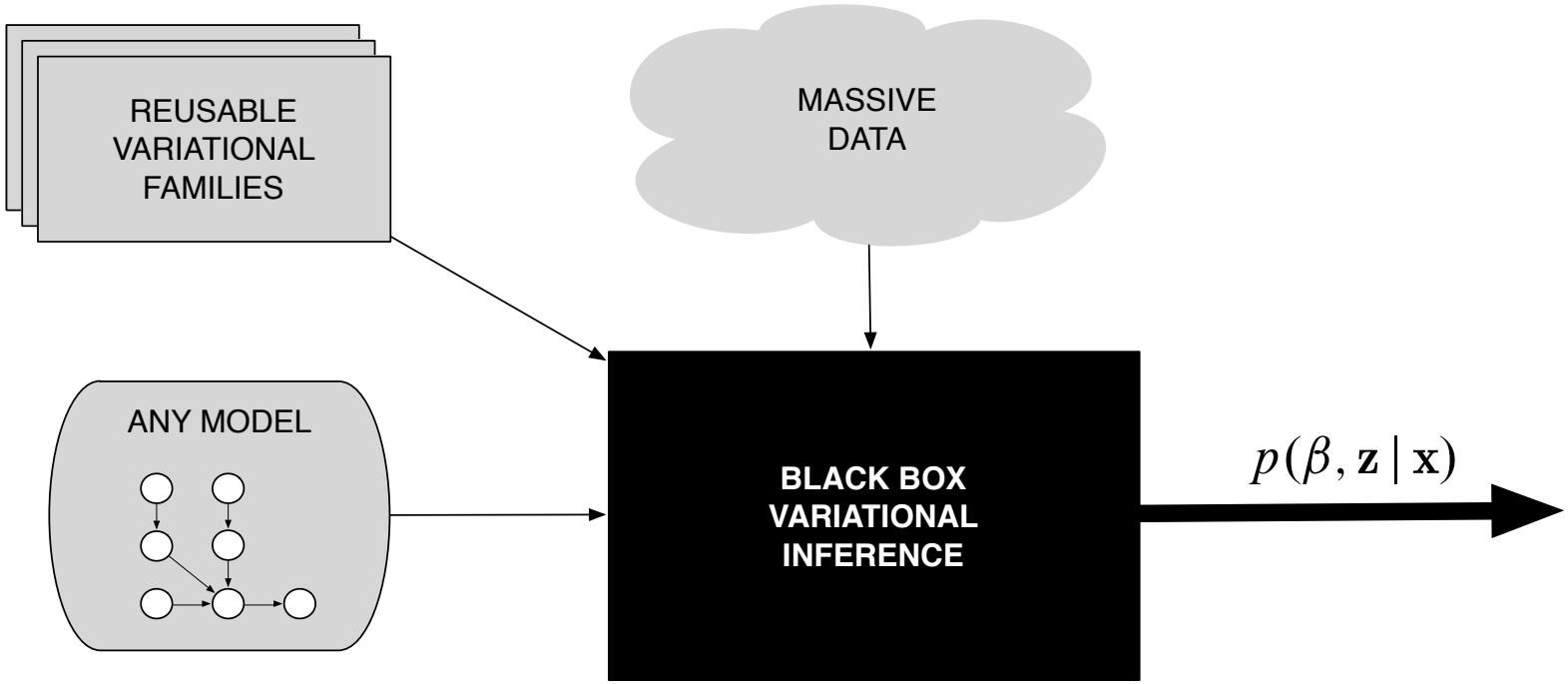
Posterior inference



$$z_{n,\ell,k} \sim \textsc{Exp-Fam}(g(\mathbf{w}_{\ell,k}^\top \mathbf{z}_{n,\ell+1}))$$

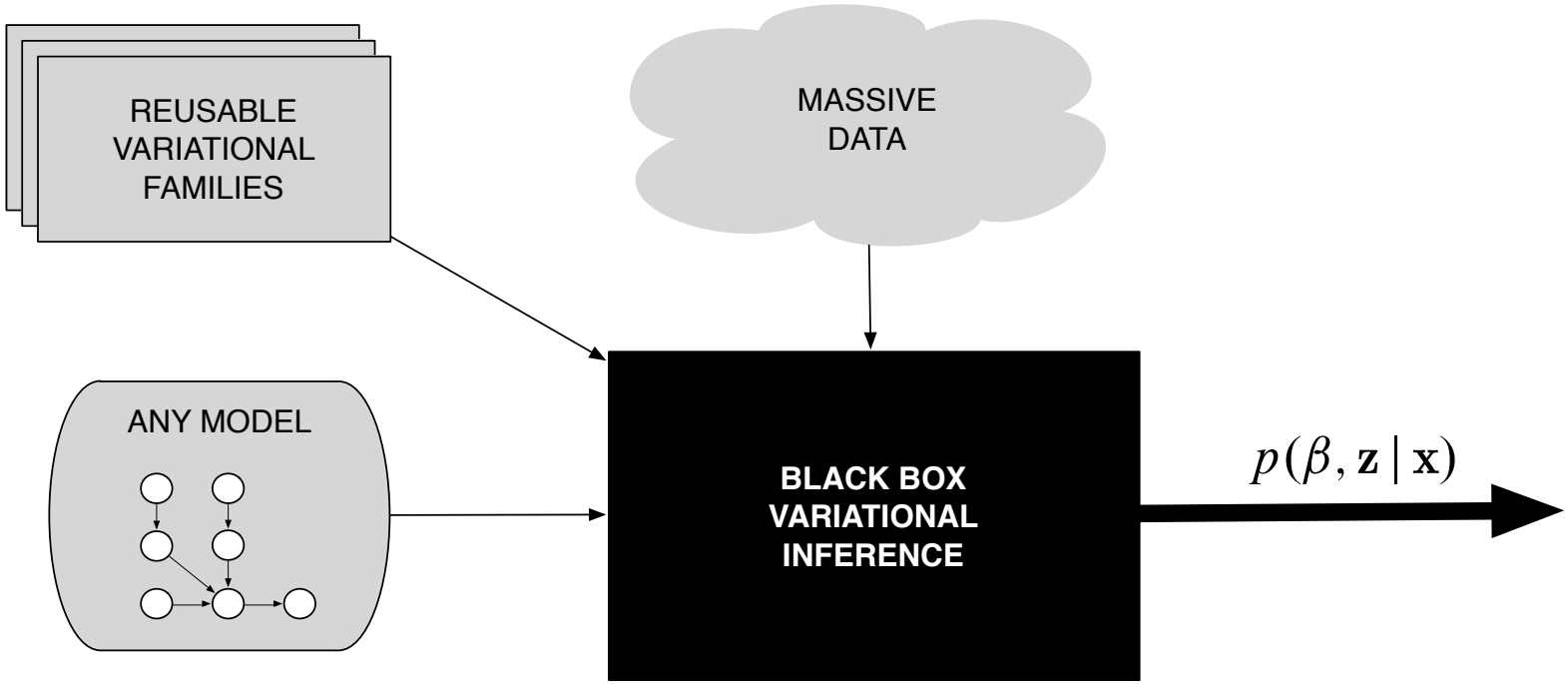
- Goal: Try out many DEFs on a dataset
  - Explore types of representations, link functions, number of layers
- Solution: **black box variational inference** (BBVI)

Black box variational inference



- Easily use variational inference with **any model**
- Perform inference with **massive data**
- **No mathematical work** beyond specifying the model

Black box variational inference



- Sample from $q(\cdot)$ (or a related distribution)
- Form noisy gradients (without model-specific computation)
- Use stochastic optimization

Black box variational inference

- BBVI with the score function estimator
- BBVI with the reparameterization gradient
- Probabilistic programming and autodifferentiation VI
- How to derive BBVI

Black box variational inference

- **BBVI with the score gradient**
- BBVI with the reparameterization gradient
- Probabilistic programming and autodifferentiation VI
- How to derive BBVI

BBVI with the score gradient

$$\nabla_{\nu} \mathcal{L} = \mathbb{E}_{q(\mathbf{z};\nu)}[\underbrace{\nabla_{\nu} \log q(\mathbf{z};\nu)}_{\text{score function}} \underbrace{(\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\nu))}_{\text{instantaneous ELBO}}]$$

- Write the gradient as an expectation.
- Use Monte Carlo to form stochastic gradients.
- Sometimes called the score, likelihood ratio, or REINFORCE gradient
  [Glynn 1990; Williams 1992; Wingate+ 2013; Ranganath+ 2014; Mnih+ 2014]

Noisy unbiased gradients

- Construct noisy unbiased gradients with Monte Carlo,

$$\hat{\nabla}_{\boldsymbol{\nu}} = \frac{1}{S}\sum_{s=1}^{S} \nabla_{\boldsymbol{\nu}} \log q(\mathbf{z}_s; \boldsymbol{\nu})(\log p(\mathbf{x}, \mathbf{z}_s) - \log q(\mathbf{z}_s; \boldsymbol{\nu})),$$

$$\text{where } \mathbf{z}_s \sim q(\mathbf{z}; \boldsymbol{\nu})$$

- To compute a noisy gradient of the ELBO,
  - sample from $q(\mathbf{z})$
  - evaluate $\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z}; \boldsymbol{\nu})$
  - evaluate $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z})$

- Satisfies the **black box criteria** — no model-specific is analysis needed.

Algorithm 3: Basic Black Box Variational Inference

Input: data $\mathbf{x}$, model $p(\mathbf{z}, \mathbf{x})$.

Initialize $\boldsymbol{\nu}$ randomly.
Set ρ_j appropriately.

while *not converged* **do**

Take S samples from the variational distribution

$$\mathbf{z}[s] \sim q(\mathbf{z}; \boldsymbol{\nu}) \quad s = 1 \ldots S$$

Calculate the noisy score gradient

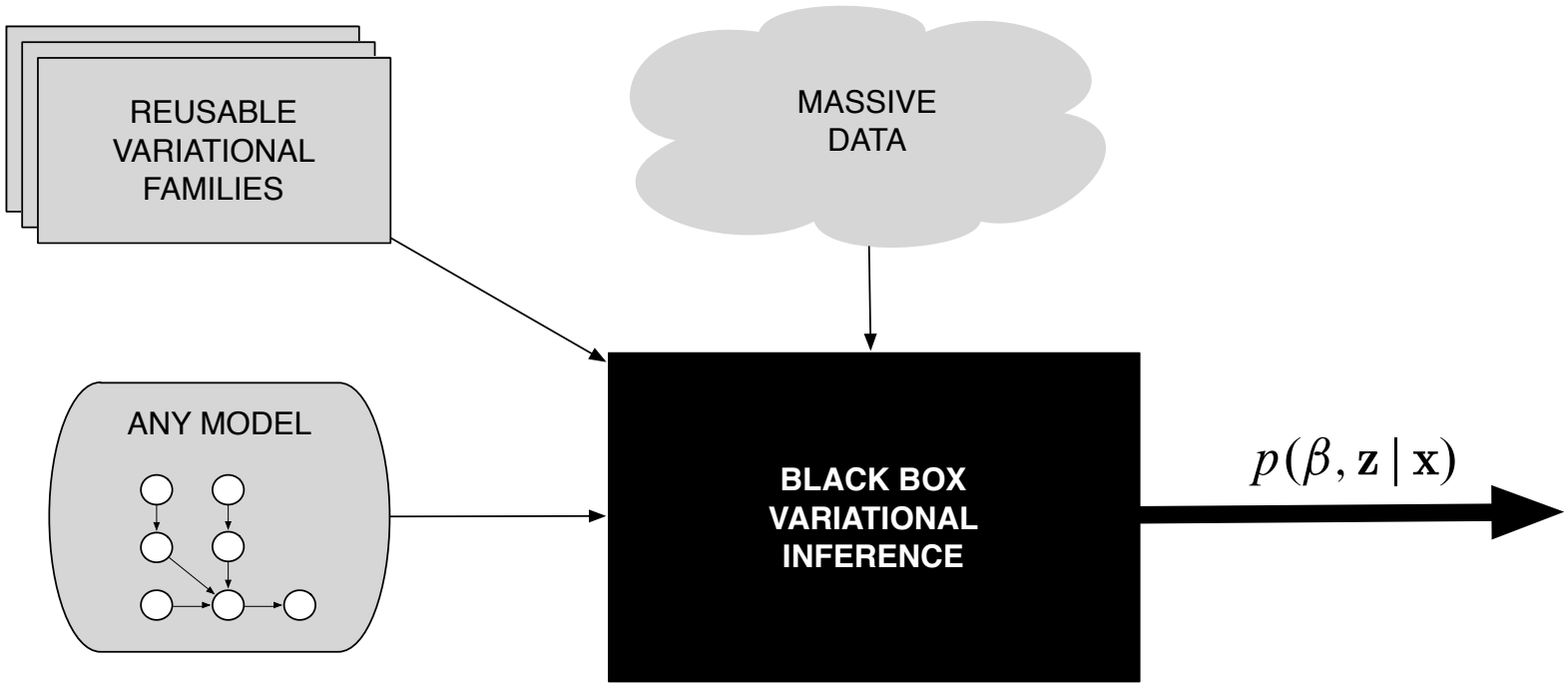
$$\tilde{g}_j = \frac{1}{S} \sum_{s=1}^{S} \nabla_{\boldsymbol{\nu}} \log q(\mathbf{z}[s]; \boldsymbol{\nu}_t)(\log p(\mathbf{x}, \mathbf{z}[s]) - \log q(\mathbf{z}[s]; \boldsymbol{\nu}_t))$$

Update the variational parameters

$$\boldsymbol{\nu}_{j+1} = \boldsymbol{\nu}_j + \rho_j \tilde{g}_j$$

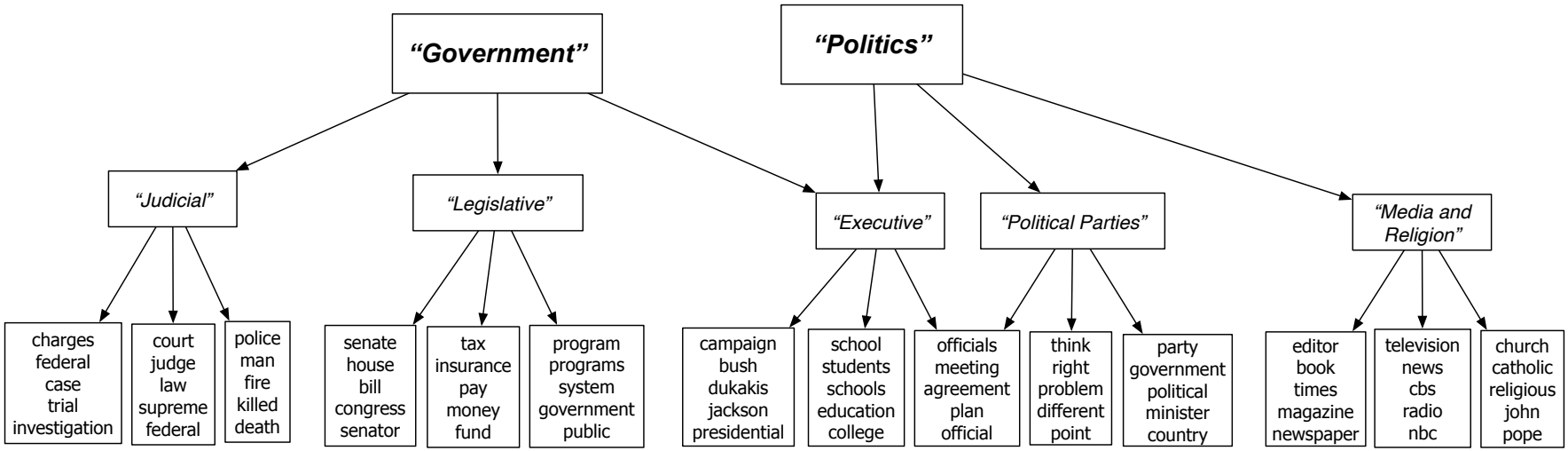
end

Black box variational inference



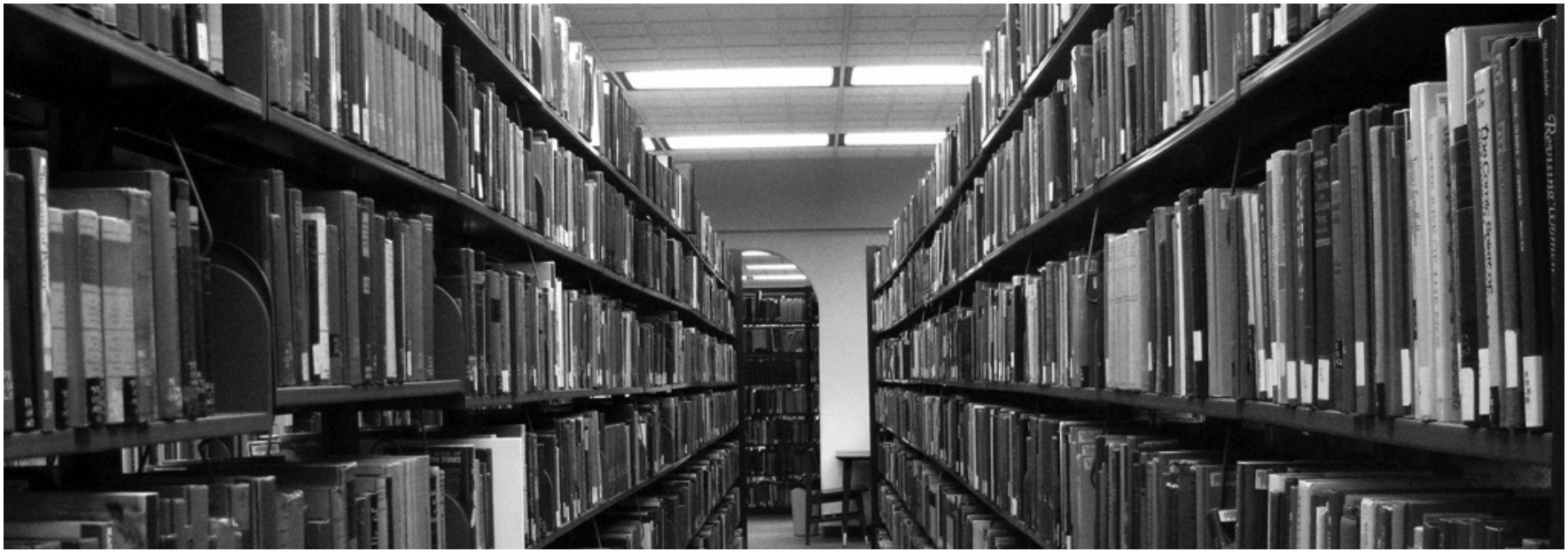
- Control the variance of the gradient
  - Rao-Blackwellization, control variates, importance sampling, ...
- Adaptive learning rates [Duchi+ 2011; Tieleman and Hinton 2012]
- Stochastic variational inference, for handling massive data

New York Times



- 160,000 documents
- 8,500 vocabulary terms
- 10M observed words

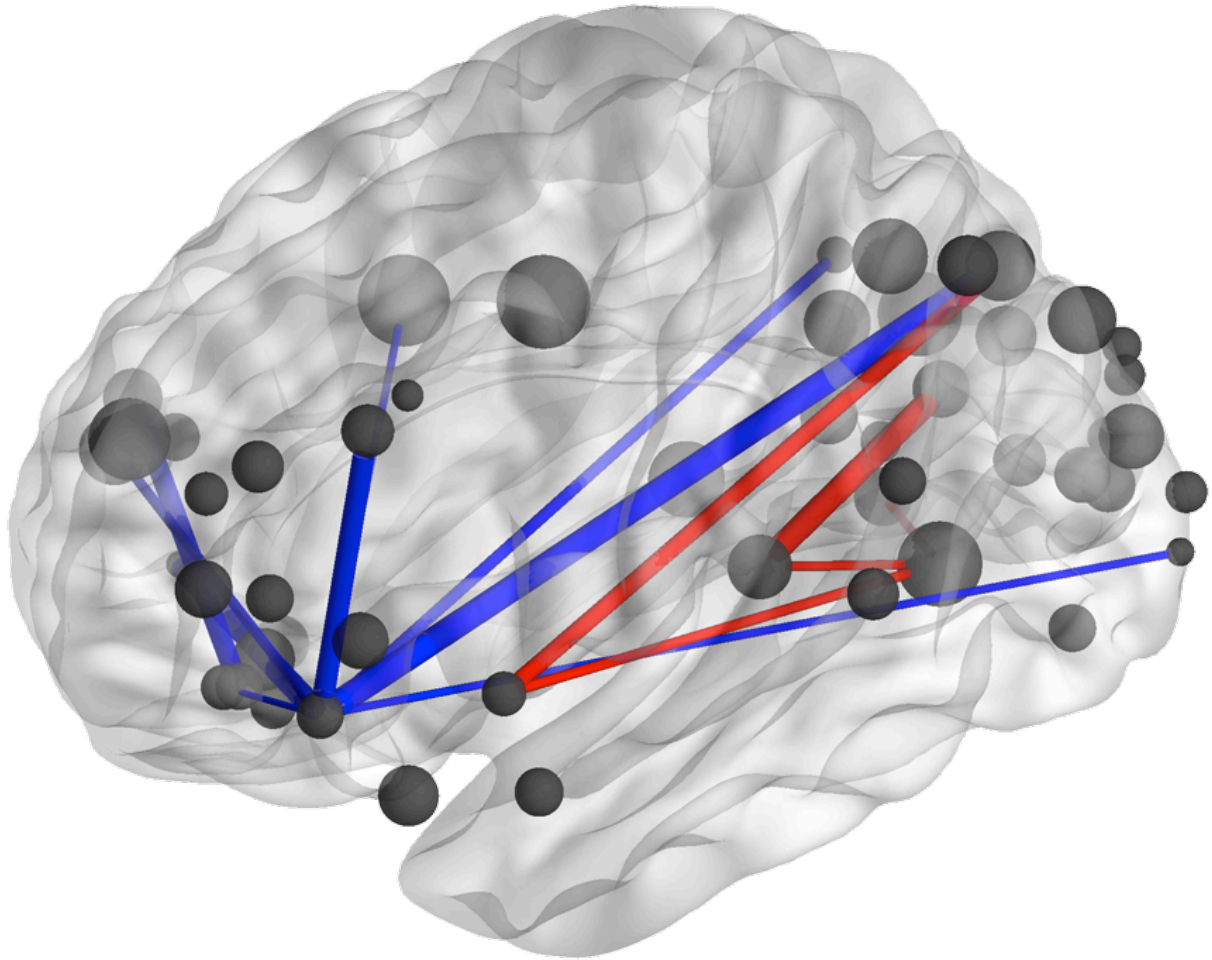
Empirical study of DEFs



- NYT and Science (about 150K documents in each, about 7K terms)
- Held-out perplexity (lower is better) [Wallach+ 2009]
- Adjusted the depth, prior on weights, and link function
- Used BBVI for all analyses

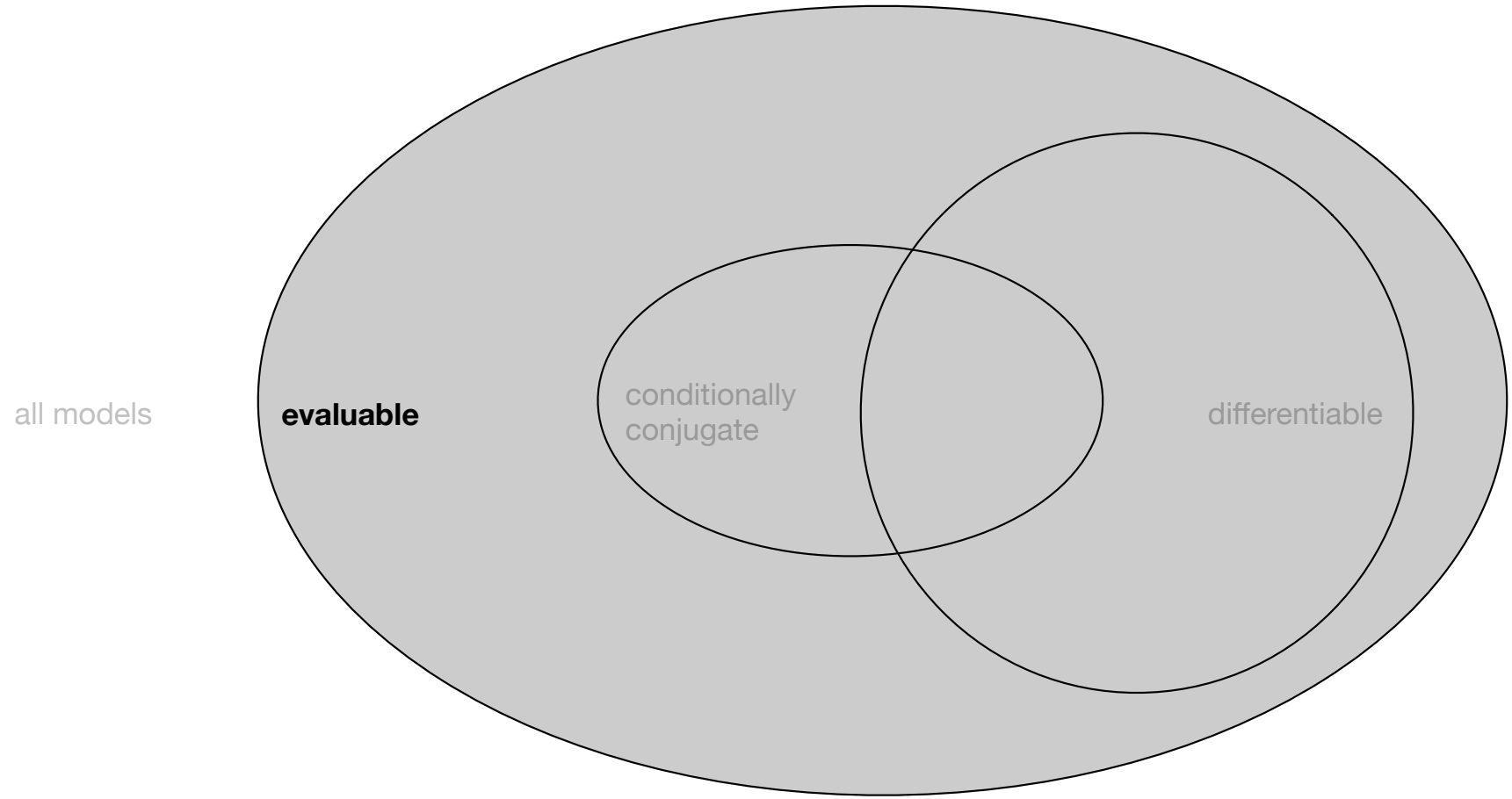
DEF evaluation

Model	$p(\mathbf{w})$	*NYT*	*Science*
LDA [Blei+ 2003]		2717	1711
DocNADE [Larochelle+ 2012]		2496	1725
Sparse Gamma 100	$\emptyset$	2525	1652
Sparse Gamma 100-30	Γ	2303	1539
Sparse Gamma 100-30-15	Γ	**2251**	1542
Sigmoid 100	$\emptyset$	2343	1633
Sigmoid 100-30	$\mathcal{N}$	2653	1665
Sigmoid 100-30-15	$\mathcal{N}$	2507	1653
Poisson 100	$\emptyset$	2590	1620
Poisson 100-30	$\mathcal{N}$	2423	1560
Poisson 100-30-15	$\mathcal{N}$	2416	1576
Poisson log-link 100-30	Γ	2288	**1523**
Poisson log-link 100-30-15	Γ	2366	1545



Neuroscience analysis of 220 million fMRI measurements

[Manning+ 2014]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Black box variational inference

- BBVI with the score function estimator
- **BBVI with the reparameterization gradient**
- Probabilistic programming and autodifferentiation VI
- How to derive BBVI

Shopper (another digression)

- Economists want to understand how people choose items
- SHOPPER is a Bayesian model of consumer behavior [Ruiz+ 2017] .
- Use it to understand patterns of purchasing behavior and estimate the effects of interventions (e.g., on price)

Shopper

- Each customer walks into the store and sequentially chooses items, each time maximizing utility. This leads to a joint:

$$p(\mathbf{y}_t) = p(y_{t1})p(y_{t2}\,|\,y_{t1})\cdots p\left(y_{tn}\,|\,\mathbf{y}_t^{[n-1]}\right).$$

- The customer picks each item conditional on features of the other items. These features capture that, e.g.,
  - medialuna and coffee go well together
  - a customer doesn't need to buy four different types of dolce de leche
  - chimichurri sauce goes on *everything*

- But these features are latent!

Shopper

- The conditional probability of picking item c is a log linear model

$$p(y_{ti} = c \,|\, \text{previously selected items}) \propto \exp\{\Psi_{tc}\}.$$

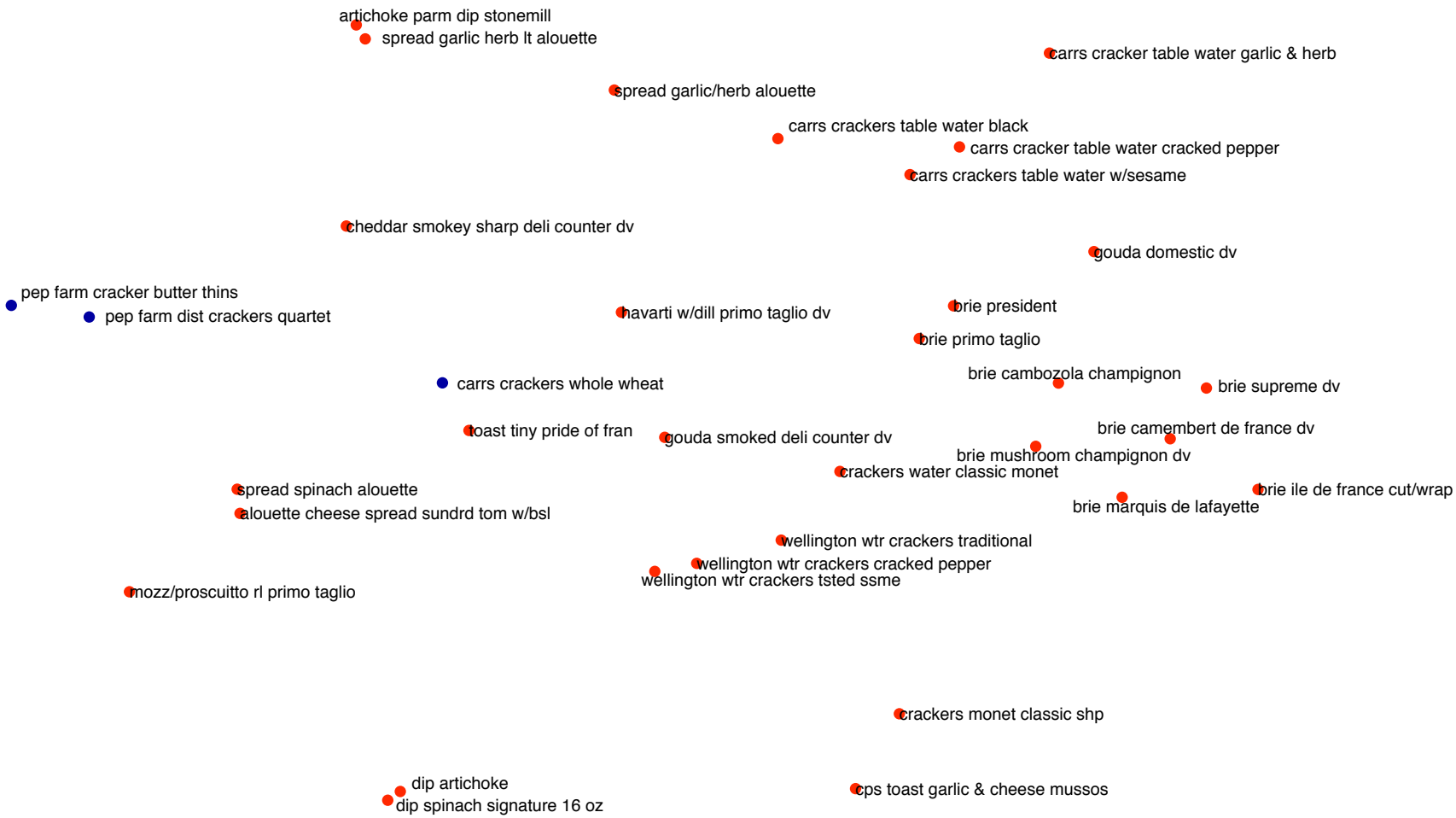
- The parameter is

$$\Psi_{tc} = \rho_c^\top \left(\sum_{j=1}^{i-1} \alpha_{y_{tj}} \right)$$

- This is an *embedding method* [Bengio+ 2003, Rudolph+ 2016] .
  - α_{dolce} : (latent) attributes of dolce de leche
  - ρ_{coffee} : attributes that go well with coffee

Shopper

- From a dataset of shopping trips, infer the posterior $p(\boldsymbol{\alpha}, \boldsymbol{\rho} \mid \mathbf{y})$.
- Posterior of per-item attributes and per-item interaction coefficients
- 3,200 customers; 5,600 items; 570K trips; 5.7M purchased items



SHOPPER on 5.7M purchases.

[more results in Ruiz+ 2017]

Shopper

- We can evaluate $\log p(\boldsymbol{\alpha}, \boldsymbol{\rho}, \mathbf{y})$
- And we can evaluate its gradient $\nabla_{\boldsymbol{\alpha},\boldsymbol{\rho}} \log p(\boldsymbol{\alpha}, \boldsymbol{\rho}, \mathbf{y})$.
- We can use *the reparameterization gradient*.

Differentiable models

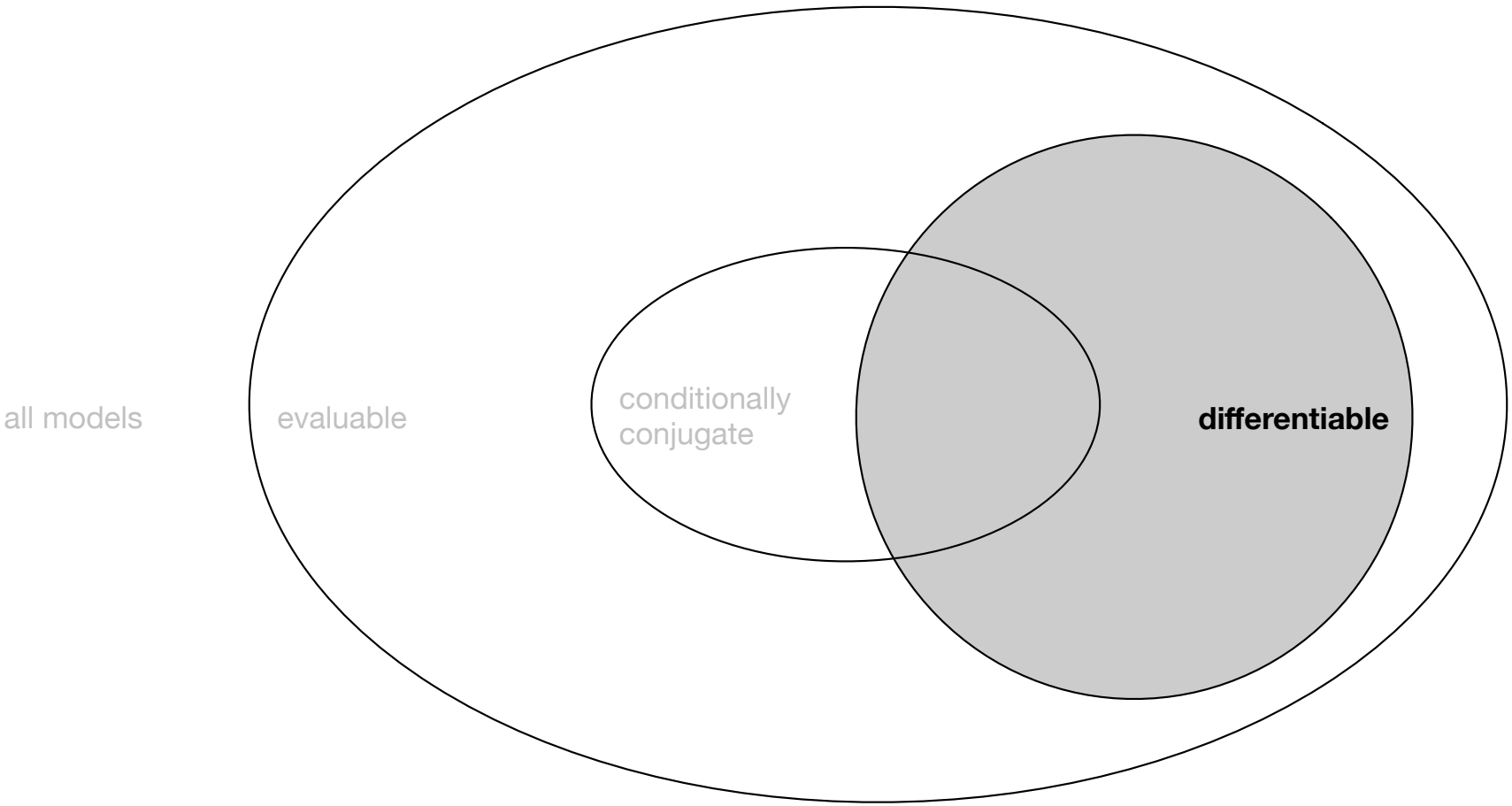
- Assume that we can express the variational distribution with a transformation, where

$$\begin{aligned}\boldsymbol{\epsilon} &\sim s(\boldsymbol{\epsilon}) \\ \mathbf{z} &= t(\boldsymbol{\epsilon}, \boldsymbol{\nu}) \\ &\rightarrow \mathbf{z} \sim q(\mathbf{z}; \boldsymbol{\nu})\end{aligned}$$

- For example,

$$\begin{aligned}\epsilon &\sim \text{Normal}(0, 1) \\ z &= \epsilon\sigma + \mu \\ &\rightarrow z \sim \text{Normal}(\mu, \sigma^2)\end{aligned}$$

- Also assume $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z})$ are differentiable with respect to $\mathbf{z}$


all models
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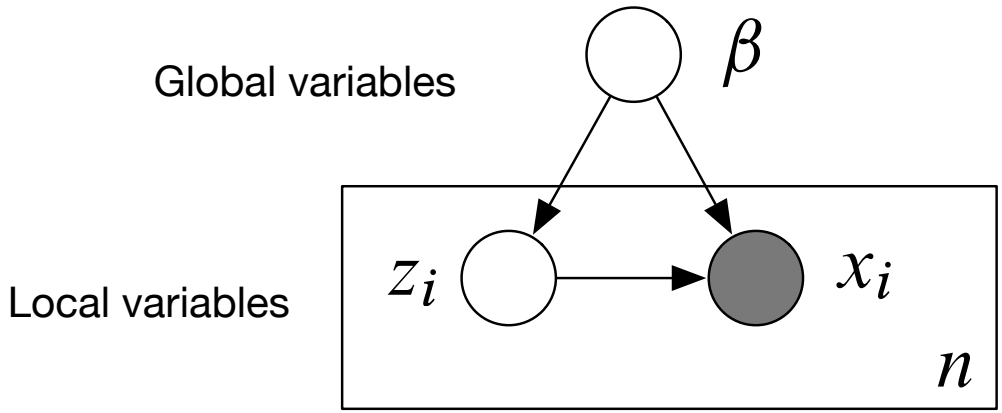
Nonconjugate models



$$p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^{n} p(z_i, x_i \mid \beta)$$

- Nonlinear time series models
- Deep latent Gaussian models
- Models with attention
- Generalized linear models
- Stochastic volatility models
- Discrete choice models
- Bayesian neural networks
- Deep exponential families
- Correlated topic models
- Sigmoid belief networks

BBVI with the reparameterization gradient

$$\nabla_{\nu}\mathcal{L} = \mathbb{E}_{s(\epsilon)}\left[\underbrace{\nabla_{\mathbf{z}}[\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\nu)]}_{\text{gradient of instananeous ELBO}} \quad \underbrace{\nabla_{\nu} t(\epsilon,\nu)}_{\text{gradient of transformation}}\right]$$

- Write the gradient as an expectation,
- Form noisy gradients with Monte Carlo.
- This is the reparameterization gradient.
  [Glasserman 1991; Fu 2006; Kingma+ 2014; Rezende+ 2014; Titsias+ 2014]

BBVI with the reparameterization gradient

$$\nabla_{\nu}\mathcal{L} = \mathbb{E}_{s(\epsilon)}\left[\underbrace{\nabla_{\mathbf{z}}[\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\nu)]}_{\text{gradient of instananeous ELBO}} \quad \underbrace{\nabla_{\nu} t(\epsilon,\nu)}_{\text{gradient of transformation}}\right]$$

- Can use autodifferentiation to take gradients (especially of the model)
- Can use and reuse different transformations [e.g., Naesseth+ 2017]
- Requires continuous latent variables

Algorithm 4: Reparameterization Black Box Variational Inference

Input: data $\mathbf{x}$, model $p(\mathbf{z}, \mathbf{x})$.

Initialize $\boldsymbol{\nu}$ randomly.
Set ρ_j appropriately.

while *not converged* **do**

Take S samples from the auxillary variable

$$\boldsymbol{\epsilon}_s \sim s(\epsilon) \quad s = 1 \ldots S$$

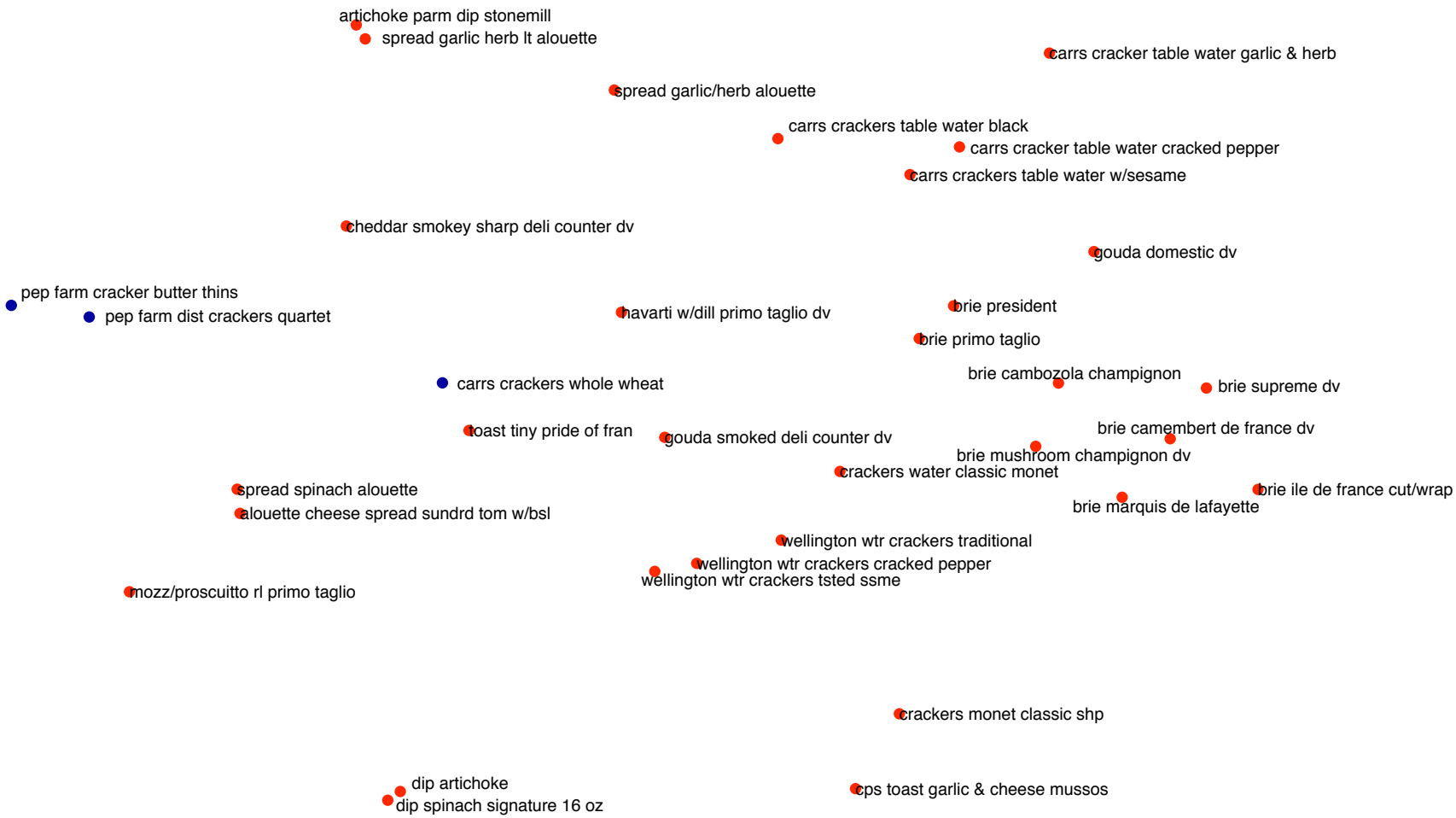
Calculate the noisy gradient

$$\tilde{g}_j = \frac{1}{S} \sum_{s=1}^{S} \nabla_{\mathbf{z}} [\log p(\mathbf{x}, t(\boldsymbol{\epsilon}_s, \boldsymbol{\nu}_n)) - \log q(t(\boldsymbol{\epsilon}_s, \boldsymbol{\nu}_n); \boldsymbol{\nu}_n)] \nabla_{\boldsymbol{\nu}} t(\boldsymbol{\epsilon}_s, \boldsymbol{\nu}_n)$$

Update the variational parameters

$$\boldsymbol{\nu}_{j+1} = \boldsymbol{\nu}_j + \rho_j \tilde{g}_j$$

end



SHOPPER on 5.7M purchases.

[more results in Ruiz+ 2017]

Score vs. reparameterization gradients

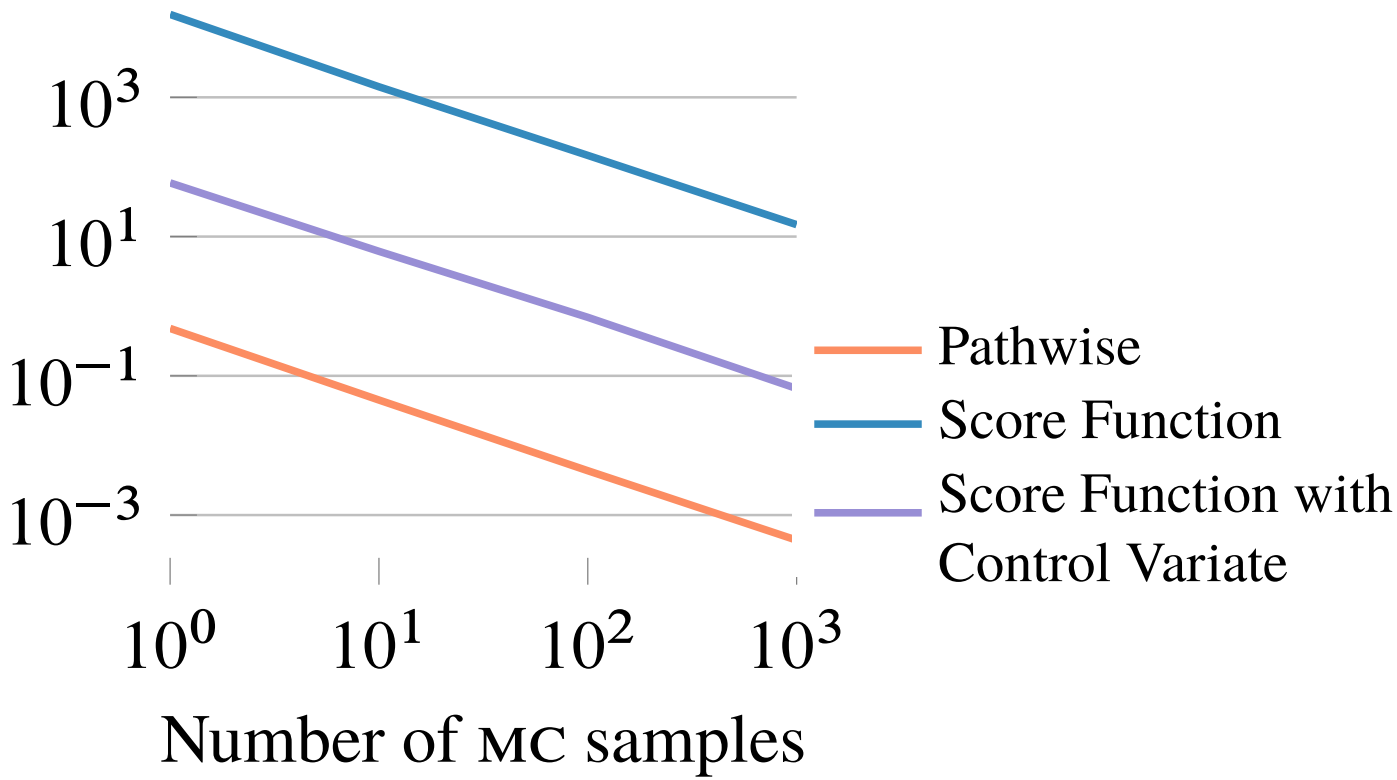
Score: $\mathbb{E}_{q(\mathbf{z};\boldsymbol{\nu})}[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu})(\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\boldsymbol{\nu}))]$

- Differentiates the variational density
- Works for discrete and continuous models
- Works for a large class of variational approximations
- Variance can be a problem

Reparameterization: $\mathbb{E}_{s(\boldsymbol{\epsilon})}[\nabla_{\mathbf{z}}[\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\boldsymbol{\nu})]\nabla_{\boldsymbol{\nu}} t(\boldsymbol{\epsilon},\boldsymbol{\nu})]$

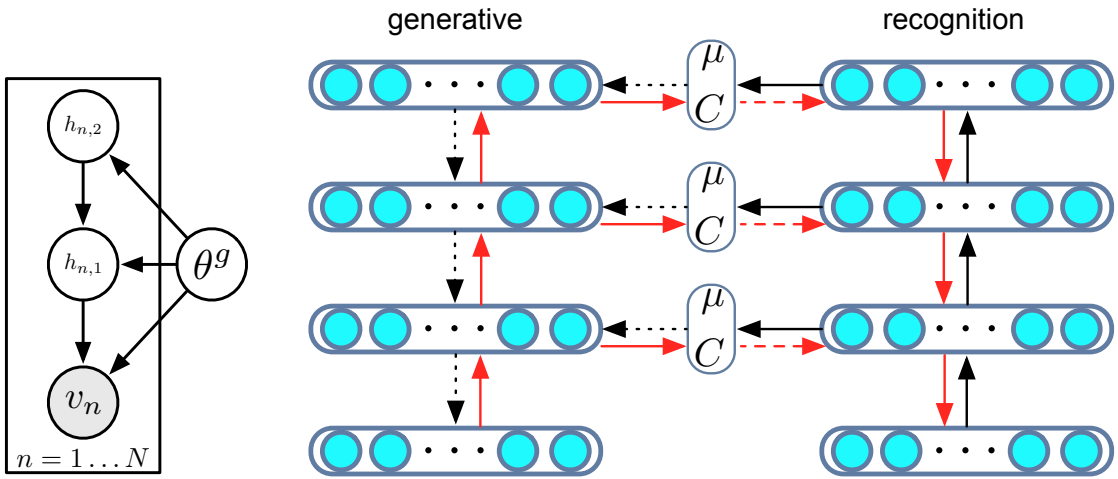
- Differentiates the instantaneous ELBO
- Requires differentiable models, i.e., no discrete variables
- Requires variational approximation to have form $\mathbf{z} = t(\boldsymbol{\epsilon},\boldsymbol{\nu})$
- Better behaved variance

Variance comparison



[Kucukelbir+ 2016]

Amortized inference and the variational autoencoder

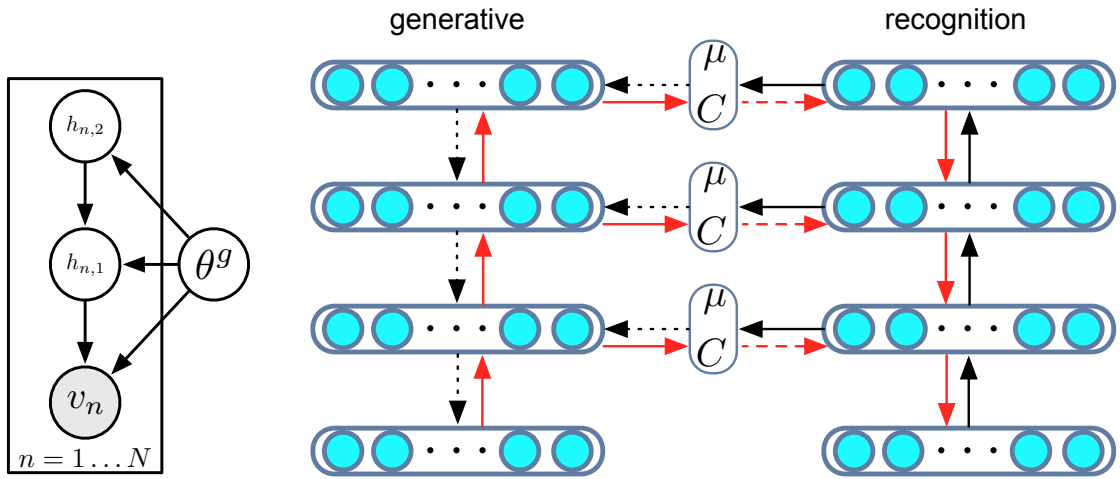


- **Amortization**:
  Variational parameters a parameterized function of the input $\nu_\eta(\mathbf{x})$
  [Gershman and Goodman 2014]

- This lets us "learn to infer." Test-time inference is fast.
  (Open question: There seems to be more to the story.)

- Plays nicely with autodifferentiation and reparameterization gradients.

Amortized inference and the variational autoencoder



- Model: Deep generative model [Kingma+ 2013; Rezende+ 2014]

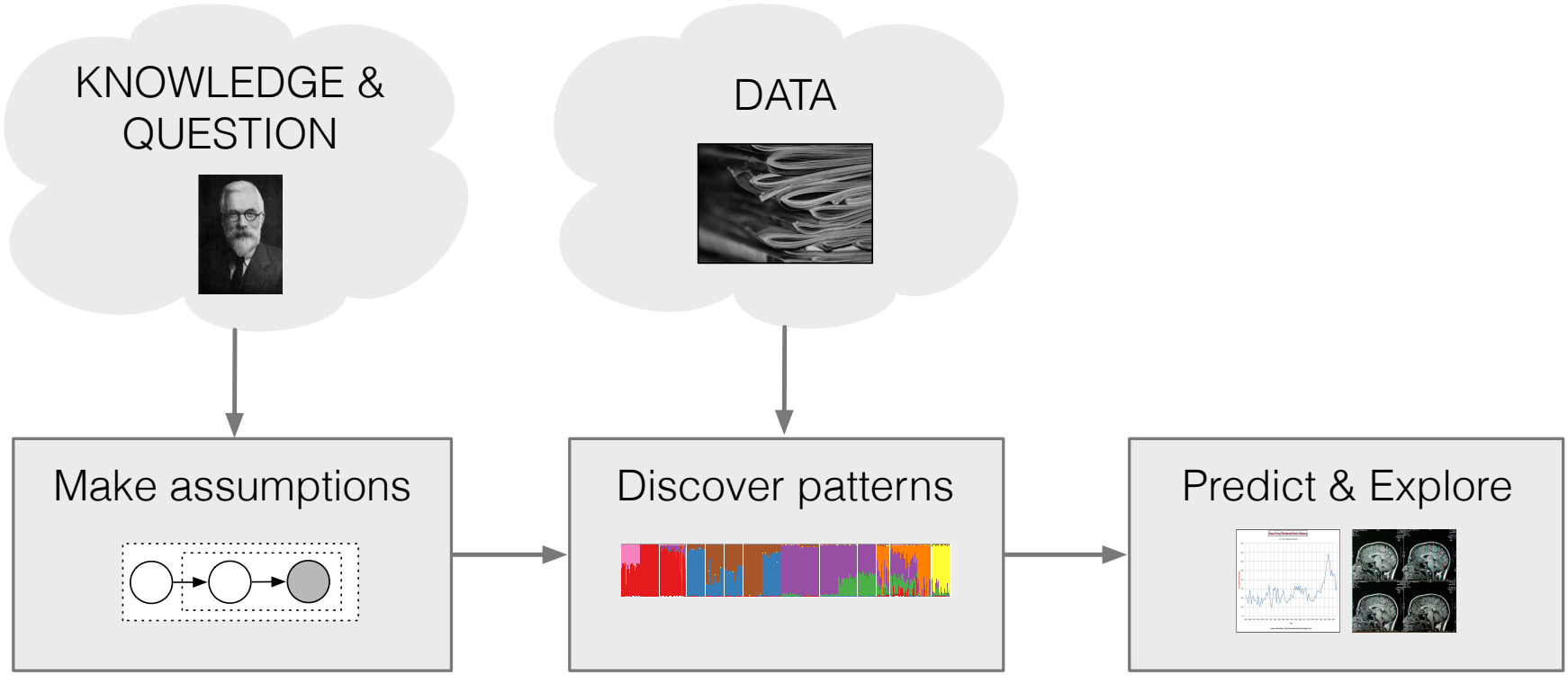
$$\mathbf{z}_i \sim \mathcal{N}(0, I)$$
$$\mathbf{x}_i \sim \mathcal{N}(f_\theta(\mathbf{z}_i), \sigma^2)$$

- Variational parameters $\boldsymbol{\nu}_\eta(\mathbf{x})$, also a deep neural network
- Algorithm:
  - Update η with reparameterization gradient
  - Update θ with gradient

Black box variational inference

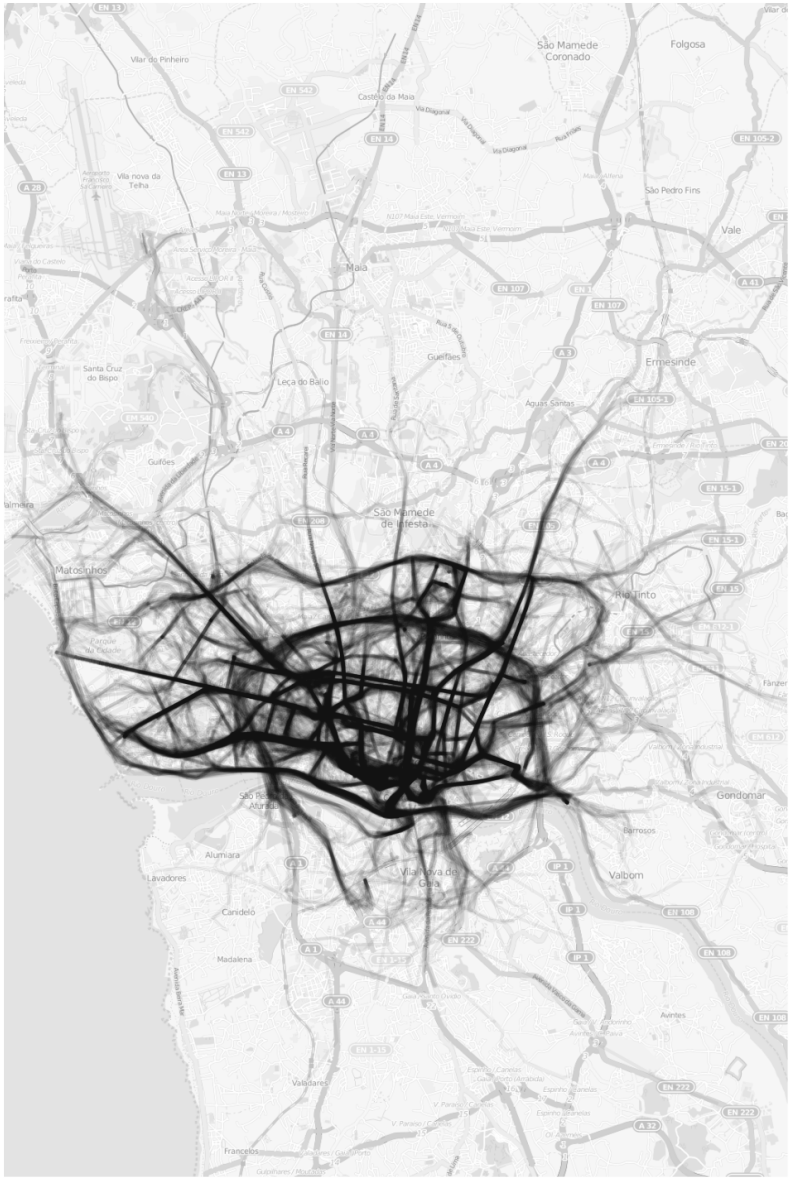
- BBVI with the score function estimator
- BBVI with the reparameterization gradient
- **Probabilistic programming and autodifferentiation VI**
- How to derive BBVI

Probabilistic programming



- Generative models are programs.
  Probabilistic programming takes this idea seriously.
- Languages for expressing models as programs
  Engines to compile models/programs to an inference executable.
- We can do this with BBVI.
  Key ideas: **autodifferentiation** and **stochastic optimization**.

Example: Taxi rides in Portugal



Example: Taxi rides in Portugal

- Data: 1.7M taxi rides in Porto, Portugal
- Multimodal probabilistic PCA with automatic relevance determination

$$
\begin{aligned}
\sigma &\sim \text{log-normal}(0, 1) \\
\\
\alpha_j &\sim \text{inv-gamma}(1, 1) && j = 1 \dots k \\
w_{x,j} &\sim \mathcal{N}(0, \sigma \cdot \alpha_j) \\
w_{y,j} &\sim \mathcal{N}(0, \sigma \cdot \alpha_j) \\
\\
z_i &\sim \mathcal{N}(0, I) && i = 1 \dots n \\
x_i &\sim \mathcal{N}(w_x^\top z_i, \sigma) \\
y_i &\sim \mathcal{N}(w_y^\top z_i, \sigma)
\end{aligned}
$$

- The generative process looks like a program.

Supervised pPCA with ARD (Stan)

```
data {
  int<lower=0> N;              // number of data points in dataset
  int<lower=0> D;              // dimension
  int<lower=0> M;              // maximum dimension of latent space to cinsider

  vector[D] x[N];
  vector[N] y;
}

parameters {
  matrix[M,N] z;               // latent variable
  matrix[D,M] w_x;             // weights parameters
  vector[M]   w_y;             // variance parameter
  real<lower=0> sigma;
  vector<lower=0>[M] alpha;    // hyper-parameters on weights
}

model {
  // priors
  to_vector(z) ~ normal(0,1);
  for (d in 1:D)
    w_x[d] ~ normal(0, sigma * alpha);
  w_y ~ normal(0, sigma * alpha);

  sigma ~ lognormal(0,1);
  alpha ~ inv_gamma(1,1);

  // likelihood
  for (n in 1:N) {
    x[n] ~ normal(w_x * col(z, n), sigma);
    y[n] ~ normal(w_y' * col(z, n), sigma);
  }
}
```


Maia
Guelfães
Ermesinde
Santa Cruz do Bispo
Leça do Balio
Aguas Santas
Guifões
São Mamede de Infesta
Matosinhos
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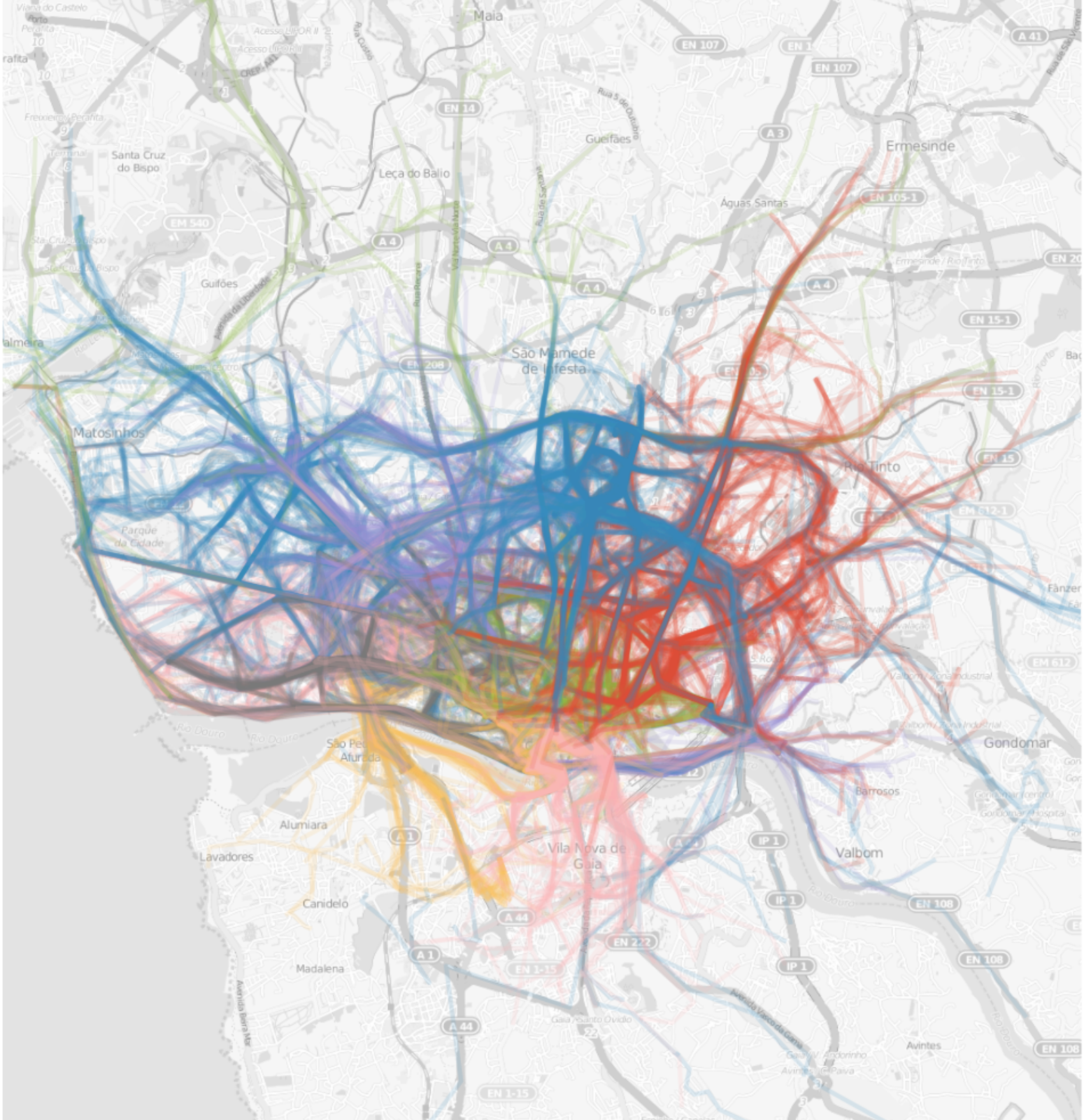
Lavadores
Vila Nova de Gaia
Valbom
Canidelo
Madalena
Avintes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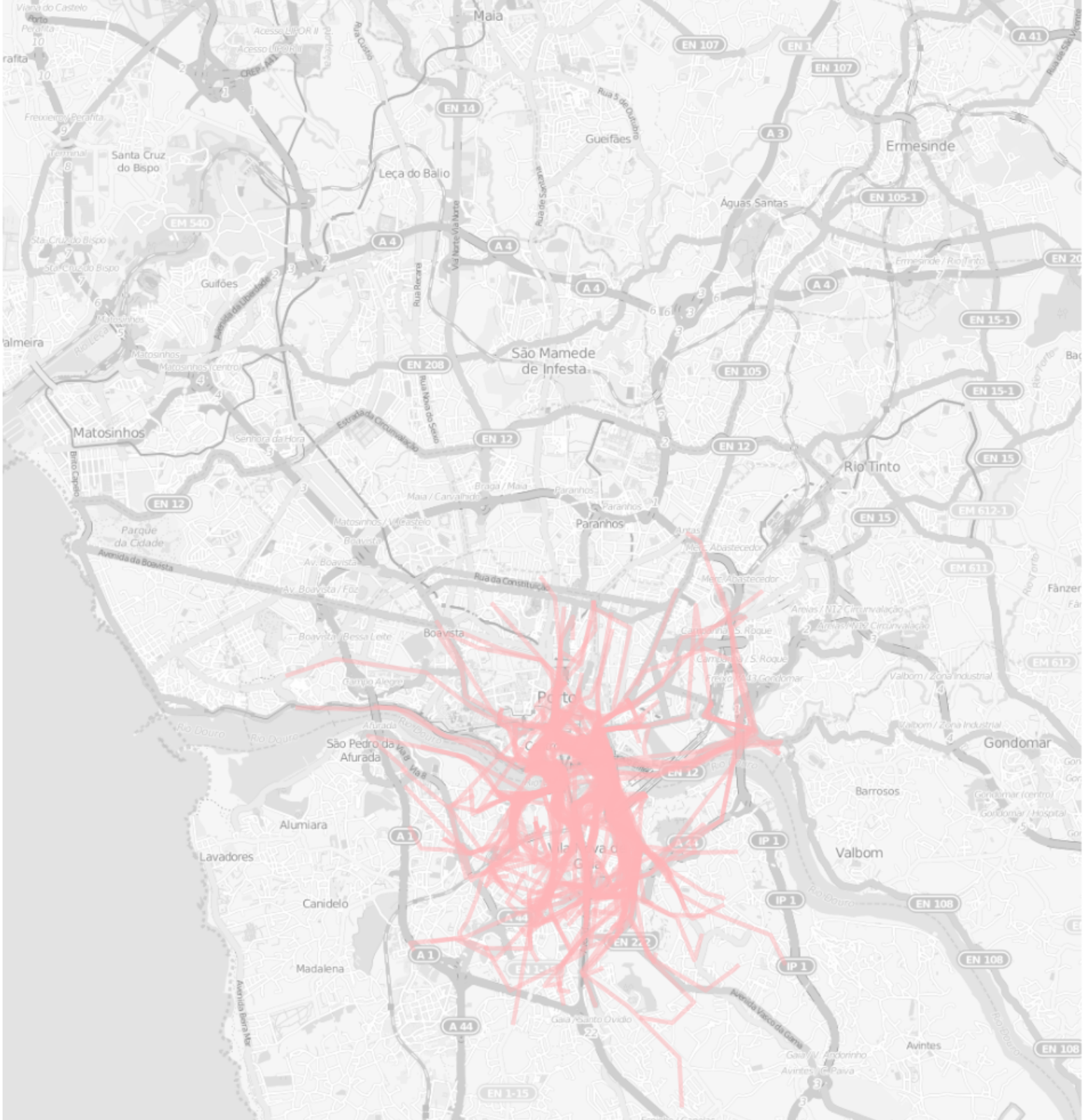
Avenida Barra Mar
Avenida Vieira de Castro
Rio Douro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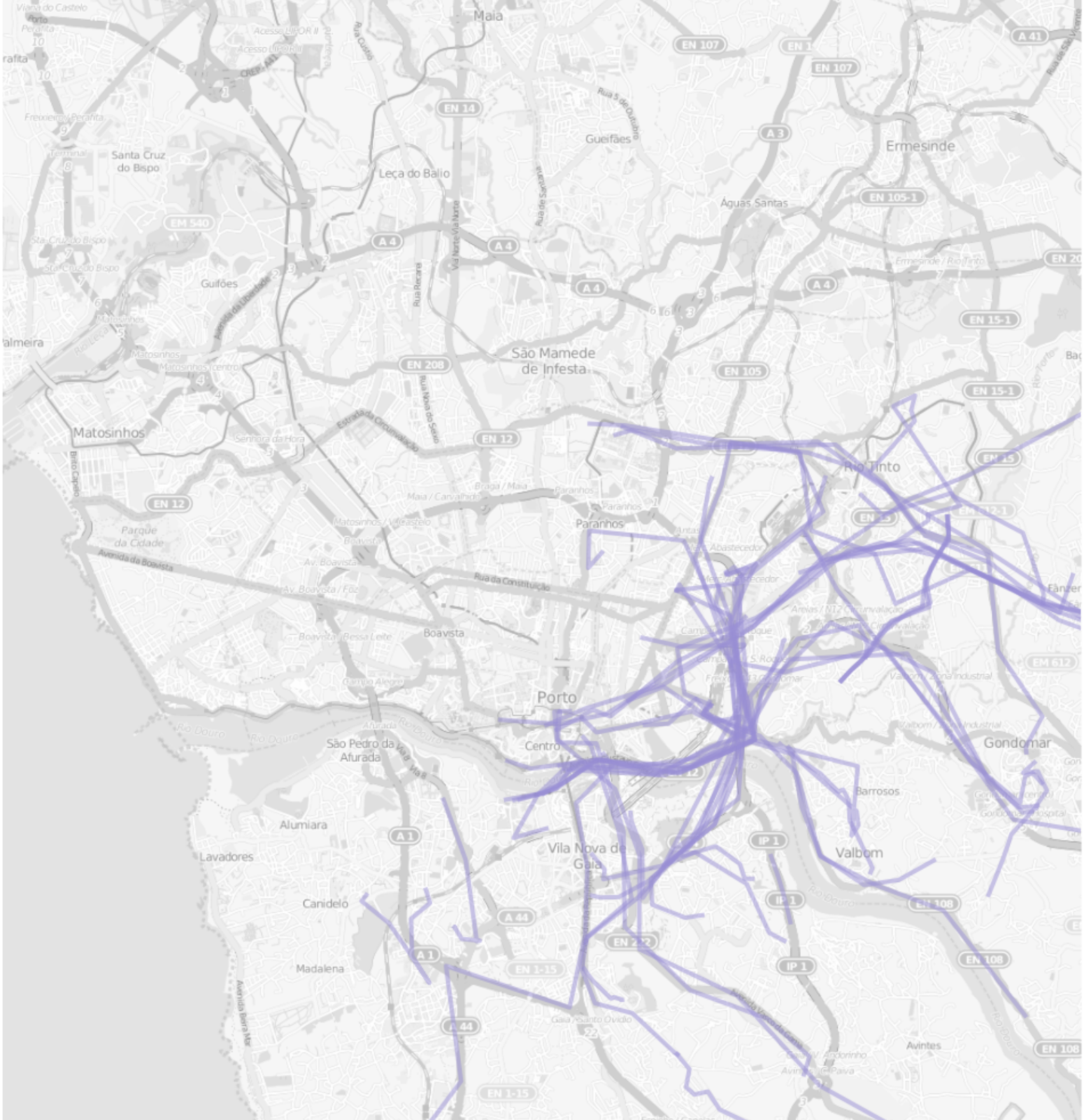
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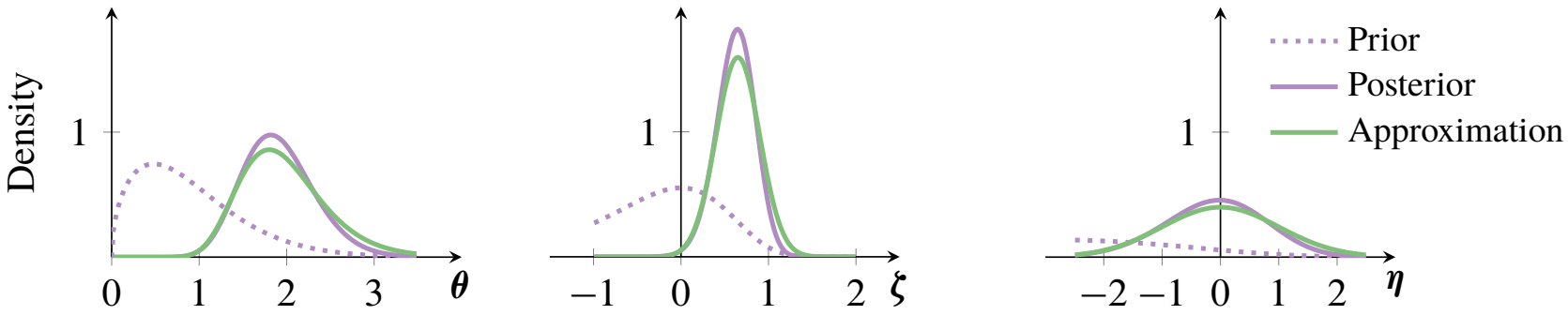
Exploring Taxi Trajectories

- Write down a supervised pPCA model (∼minutes).
- Use VI to fit the model in Stan (∼hours).
- Estimate latent representation z_i of each taxi ride (∼minutes).

- Write down a mixture model (∼minutes).
- Use VI to cluster the latent representations (∼minutes).

What would take weeks → a single day.

Automatic differentiation variational inference



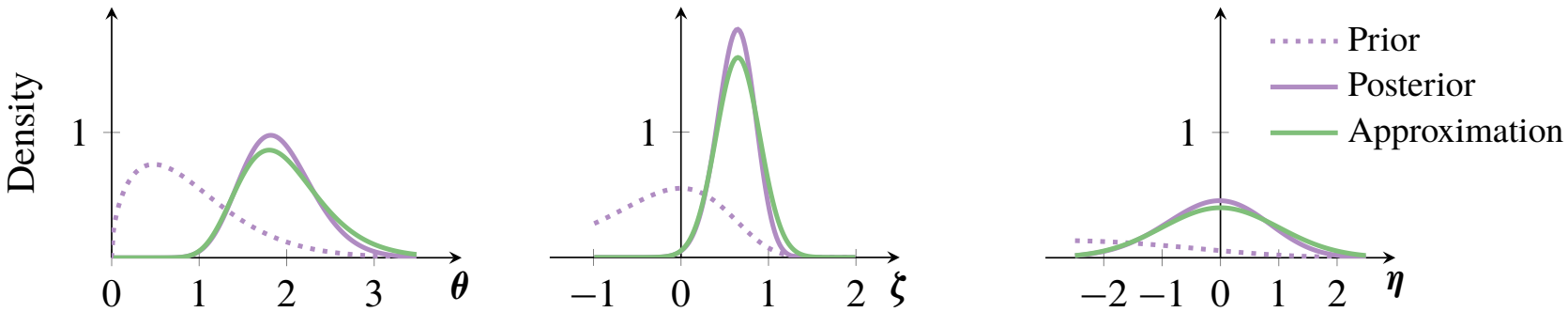
(a) Latent variable space **(b)** Real coordinate space **(c)** Standardized space

1. Transform the model.

- Transform from $p(\mathbf{z}, \mathbf{x})$ to $p(\zeta, \mathbf{x})$, where $\zeta \in \mathbb{R}^d$.
- The mapping is in the joint,

$$p(\zeta, \mathbf{x}) = p\left(\mathbf{x}, s(\zeta)\right) \left| \det J_s(\zeta) \right|.$$

Automatic differentiation variational inference



(a) Latent variable space **(b)** Real coordinate space **(c)** Standardized space

2. Redefine the variational problem.

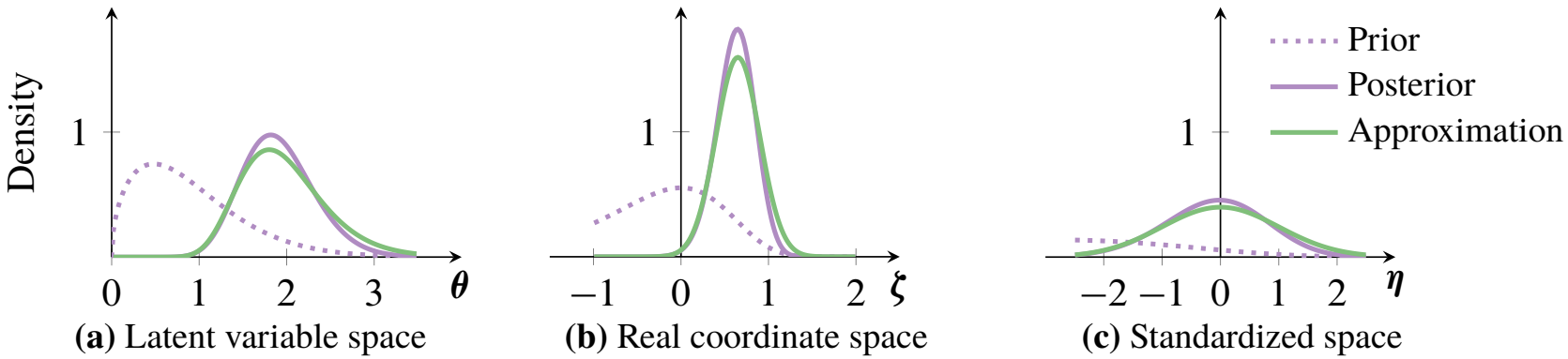
- The variational family is mean-field Gaussian

$$q(\boldsymbol{\zeta}\,;\,\boldsymbol{\nu}) = \prod_{k=1}^{K} \varphi\left(\zeta_k\,;\,\nu_k\right),$$

- The ELBO is

$$\mathscr{L} = \mathbb{E}_{q(\zeta)}\Big[\log p\left(\mathbf{x}, s(\boldsymbol{\zeta})\right) + \log\left|\det J_s(\boldsymbol{\zeta})\right|\Big] + \mathbb{H}(q)$$

Automatic differentiation variational inference

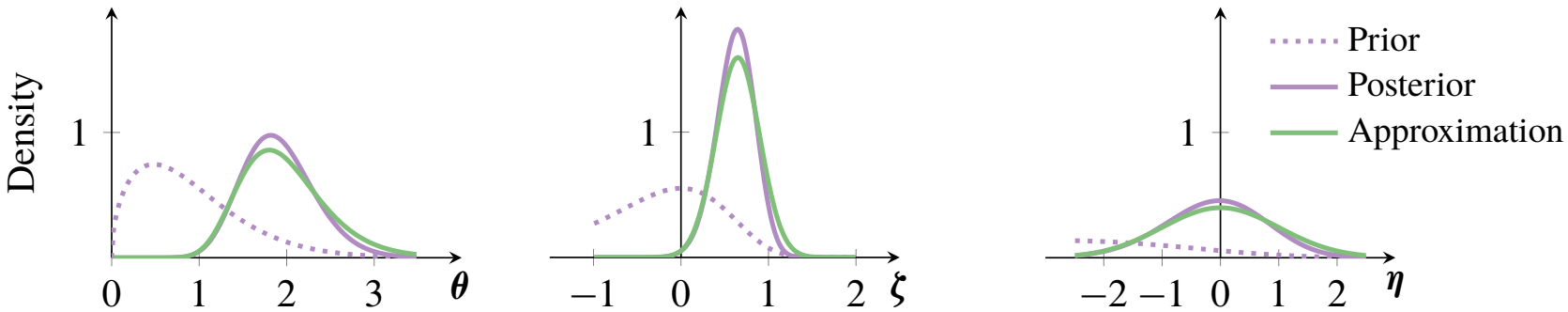


(a) Latent variable space **(b)** Real coordinate space **(c)** Standardized space

3. Use the reparameterization gradient

- Transform ζ using a standard normal $\epsilon \sim \mathcal{N}(0, \mathbf{I})$ to a general normal.
- This is a second transformation of the original latent variable.
- Autodifferentiation handles the reparameterization gradient.

Automatic differentiation variational inference



(a) Latent variable space **(b)** Real coordinate space **(c)** Standardized space

Implementation

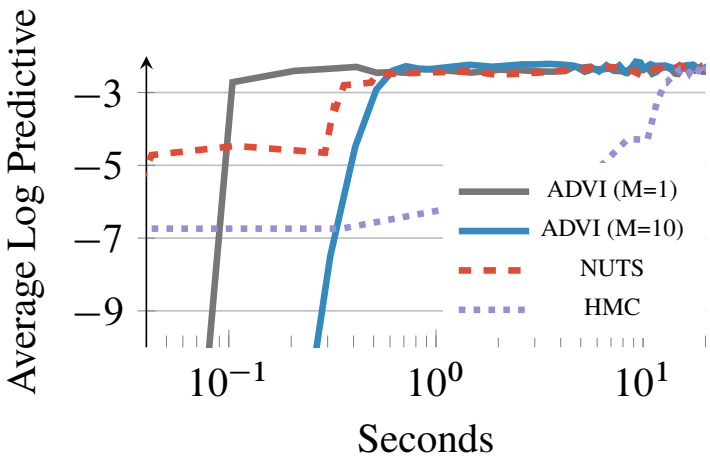
- Stan automates going from $\log p(\mathbf{x}, \mathbf{z})$ to

$$\log p(\mathbf{x}, s(\zeta)) + \log \left| \det J_s(\zeta) \right|$$

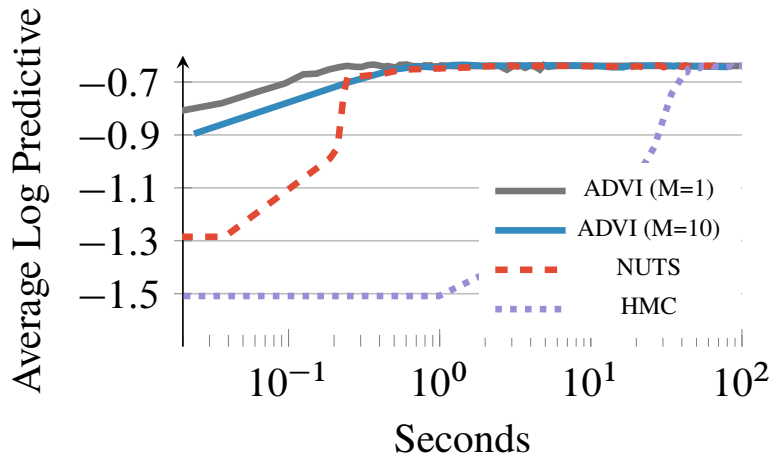
$$\nabla_\zeta (\log p(\mathbf{x}, s(\zeta)) + \log \left| \det J_s(\zeta) \right|)$$

- Use reparameterization BBVI (with the Gaussian transformation)
- Can incorporate SVI and other innovations

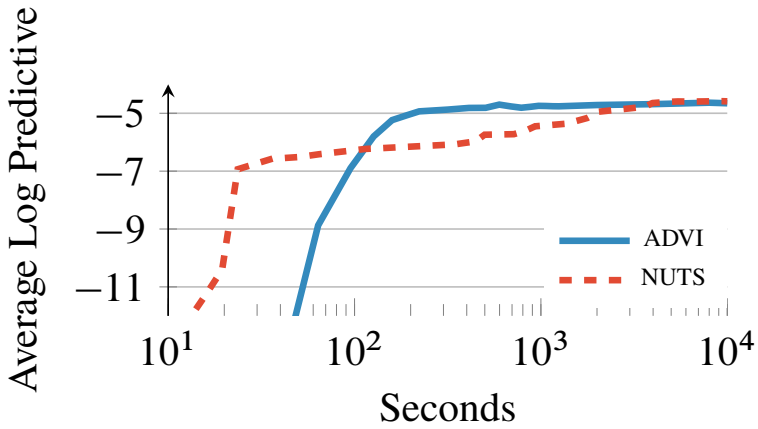
Some benchmarks



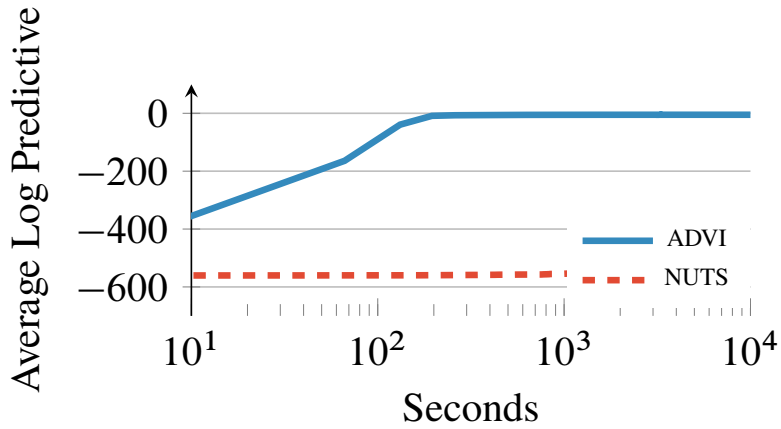
(a) Linear Regression with ARD



(b) Hierarchical Logistic Regression



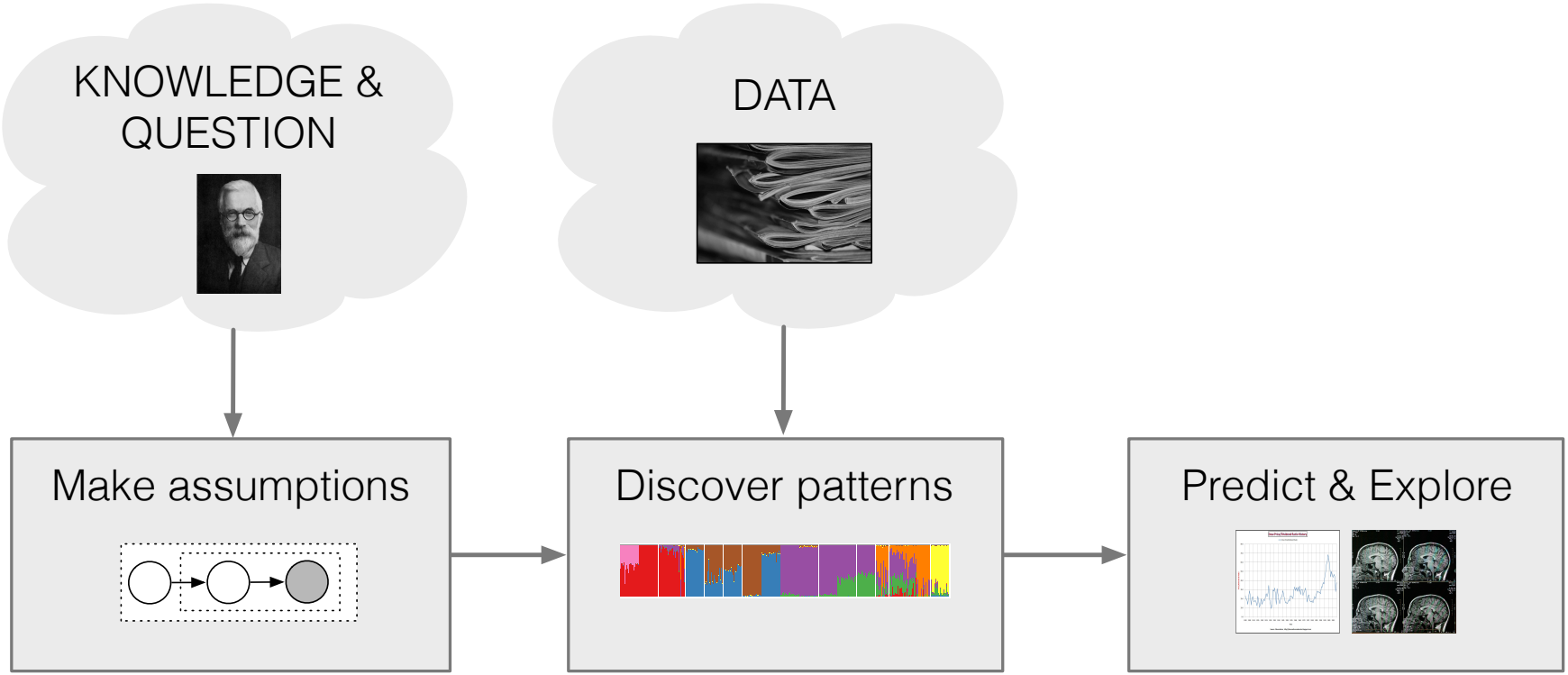
(a) Gamma Poisson Predictive Likelihood



(b) Dirichlet Exponential Predictive Likelihood

[Kucukelbir+ 2016]

Probabilistic programming



VI is part of several probabilistic programming systems:

- **Edward**: `edwardlib.org`
- **PyMC3**: `github.com/pymc-devs/pymc3`
- **Stan**: `mcstan.org`

Black box variational inference

- BBVI with the score function estimator
- BBVI with the reparameterization gradient
- Probabilistic programming and autodifferentiation VI
- **How to derive BBVI**

Score gradient

$$\nabla_{\nu}\mathcal{L} = \mathbb{E}_{q(\mathbf{z};\nu)}[\underbrace{\nabla_{\nu}\log q(\mathbf{z};\nu)}_{\text{score function}}\ \underbrace{(\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\nu))}_{\text{instantaneous ELBO}}]$$

Reparameterization gradient

$$\nabla\mathcal{L} = \mathbb{E}_{s(\epsilon)}\left[\underbrace{\nabla_{\mathbf{z}}[\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\nu)]}_{\text{gradient of instananeous ELBO}}\ \underbrace{\nabla_{\nu}t(\epsilon,\nu)}_{\text{gradient of transformation}}\right]$$

A recipe for variational inference

$$p(\mathbf{z}, \mathbf{x})$$

Posit a model, a joint distribution of hidden and observed variables.

A recipe for variational inference

$$q(\mathbf{z}; \boldsymbol{\nu})$$

Choose the variational family, distributions of the hidden variables.

A recipe for variational inference

$$\mathcal{L}(\boldsymbol{\nu}) = \mathbb{E}_{q(\mathbf{z};\boldsymbol{\nu})}[\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\boldsymbol{\nu})]$$

Write the ELBO, the objective function for finding a $q(\mathbf{z};\boldsymbol{\nu})$ close to $p(\mathbf{z}|\mathbf{x})$.

A recipe for variational inference

$$\mathscr{L}(v) = x v^2 + \log v \quad \text{(example)}$$

Integrate: The ELBO is a function of data and variational parameters.

A recipe for variational inference

$$\nabla_v \mathcal{L}(\boldsymbol{v}) = 2x\boldsymbol{v} + 1/\boldsymbol{v} \quad \text{(example)}$$

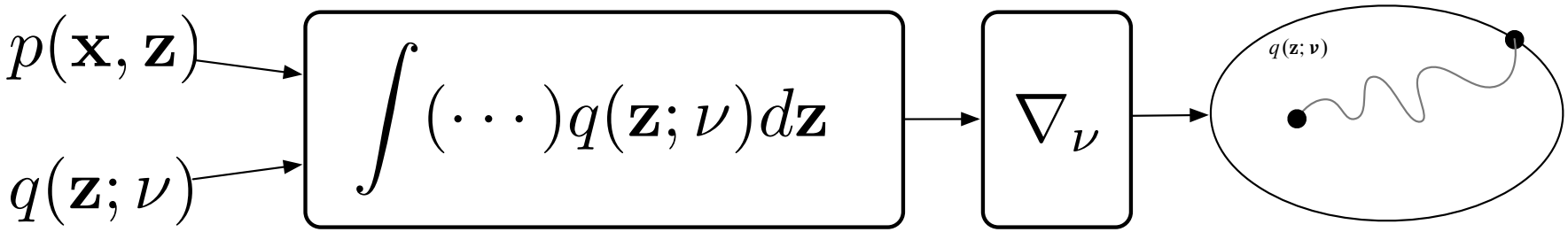
Take derivatives.

A recipe for variational inference

$$\boldsymbol{\nu}_{t+1} = \boldsymbol{\nu}_t + \rho_t \nabla_{\boldsymbol{\nu}} \mathcal{L}$$

Optimize.

A recipe for variational inference



1. Posit a model
2. Choose a variational family
3. Integrate (calculate the ELBO)
4. Take derivatives
5. Optimize

Bayesian logistic regression

- Data are pairs (x_i, y_i)
  - x_i is a covariate
  - $y_i \in \{0, 1\}$ is a binary label
  - z are the regression coefficients

- Conditional on covariates, Bayesian LR posits a generative process of labels

$$z \sim N(0, 1)$$
$$y_i \,|\, x_i, z \sim \text{Bernoulli}(\sigma(z x_i)),$$

  where $\sigma(\cdot)$ is the logistic function, mapping reals to $(0, 1)$.

VI for Bayesian logistic regression

- Consider one data point (x, y).
- Our goal is to approximate the posterior coefficient $p(z \mid x, y)$.
- The variational family $q(z; \boldsymbol{\nu})$ is a normal; $\boldsymbol{\nu} = (\mu, \sigma^2)$
- The ELBO is

$$\mathcal{L}(\mu, \sigma^2) = \mathbb{E}_q[\log p(z) + \log p(y \mid x, z) - \log q(z)]$$

VI for Bayesian logistic regression

$$\mathcal{L}(\mu, \sigma^2) \quad = \quad \mathbb{E}_q[\log p(z) - \log q(z) + \log p(y \mid x, z)]$$

VI for Bayesian logistic regression

$$
\begin{aligned}
\mathcal{L}(\mu, \sigma^2) &= \mathbb{E}_q[\log p(z) - \log q(z) + \log p(y \mid x, z)] \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_q[\log p(y \mid x, z)] + C
\end{aligned}
$$

VI for Bayesian logistic regression

$$
\begin{aligned}
\mathcal{L}(\mu, \sigma^2) &= \mathbb{E}_q[\log p(z) - \log q(z) + \log p(y \mid x, z)] \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_q[\log p(y \mid x, z)] + C \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_q[yxz - \log(1 + \exp(xz))]
\end{aligned}
$$

VI for Bayesian logistic regression

$$
\begin{aligned}
\mathcal{L}(\mu, \sigma^2) &= \mathbb{E}_q[\log p(z) - \log q(z) + \log p(y \mid x, z)] \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_q[\log p(y \mid x, z)] + C \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_q[yxz - \log(1 + \exp(xz))] \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + yx\mu - \mathbb{E}_q[\log(1 + \exp(xz))]
\end{aligned}
$$

VI for Bayesian logistic regression

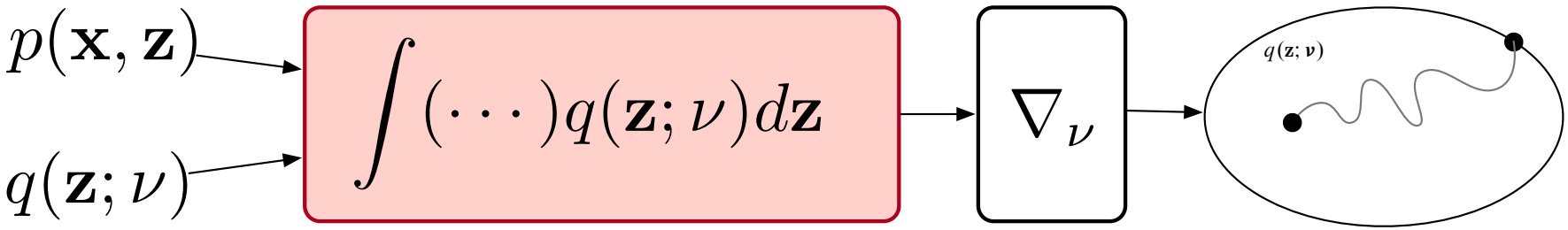
$$
\begin{aligned}
\mathcal{L}(\mu, \sigma^2) &= \mathbb{E}_q[\log p(z) - \log q(z) + \log p(y \mid x, z)] \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_q[\log p(y \mid x, z)] + C \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_q[yxz - \log(1 + \exp(xz))] \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + yx\mu - \mathbb{E}_q[\log(1 + \exp(xz))]
\end{aligned}
$$

We are stuck—we cannot analytically take the expectation.

Options?

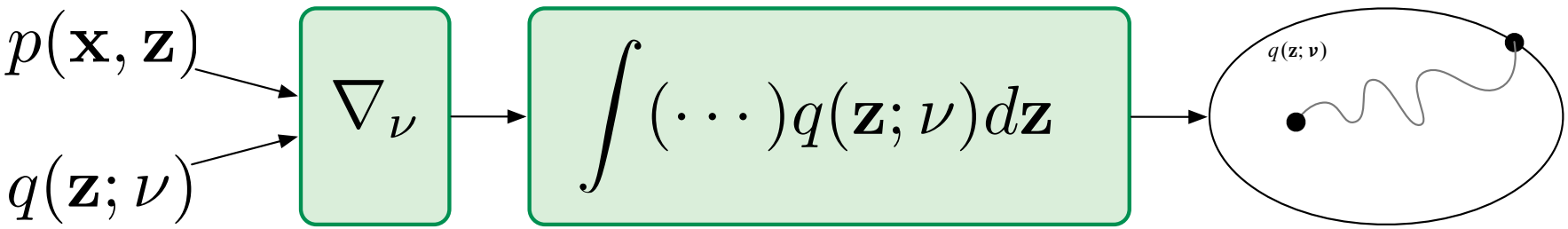
- Derive a model-specific bound
  [Jordan and Jaakola 1996], [Braun and McAuliffe 2008], others
- Use other approximations (that require model-specific analysis)
  [Wang and Blei 2013], [Knowles and Minka 2011]
- But neither satisfies the *black box criteria*.

The problem with the VI recipe



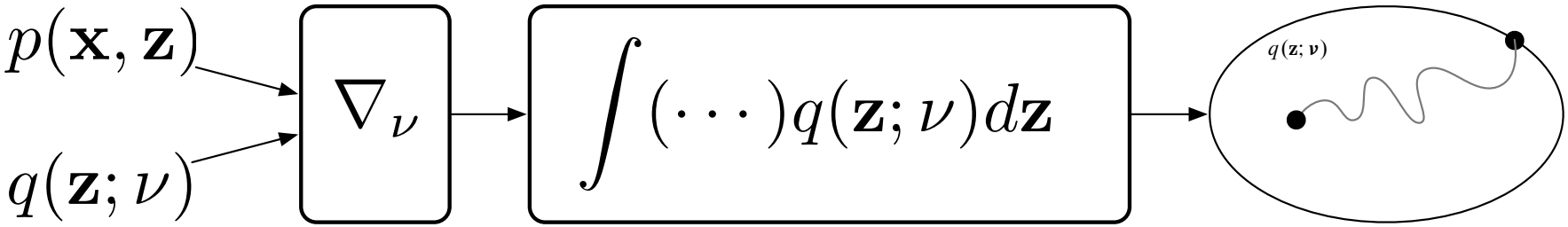
The integral is hard to take.

Solution: Swap integration and differentiation



Swap! Now we can use MC gradients and stochastic optimization.

The new recipe



- This is the key idea behind modern methods in variational inference
- It has enabled score gradients, reparameterization gradients, amortized inference, probabilistic programming, complex variational families, and alternative divergences.
- How do we reverse differentiation and integration?

Reversing the gradient and the expectation

- Denote the *instantaneous ELBO*

$$g(\mathbf{z}, \boldsymbol{\nu}) = \log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}; \boldsymbol{\nu}).$$

- The ELBO is its expectation

$$\mathscr{L} = \mathbb{E}_q \left[g(\mathbf{z}, \boldsymbol{\nu}) \right] = \int q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z}$$

- We want to calculate $\nabla_{\boldsymbol{\nu}} \mathscr{L}$.

Reversing the gradient and the expectation

Fact:

$$\nabla_{\boldsymbol{\nu}} q(\mathbf{z}; \boldsymbol{\nu}) = q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\boldsymbol{\nu}} \log q(\mathbf{z}; \boldsymbol{\nu}).$$

Reversing the gradient and the expectation

Fact:

$$\nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) = q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}).$$

With this,

$$\nabla_{\nu} \mathcal{L} \quad = \quad \nabla_{\nu} \int q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z}$$

Reversing the gradient and the expectation

Fact:

$$\nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) = q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}).$$

With this,

$$\begin{aligned} \nabla_{\nu} \mathcal{L} &= \nabla_{\nu} \int q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\ &= \int \nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \end{aligned}$$

Reversing the gradient and the expectation

Fact:

$$\nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) = q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}).$$

With this,

$$\begin{aligned}
\nabla_{\nu} \mathcal{L} &= \nabla_{\nu} \int q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\
&= \int \nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\
&= \int q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z}
\end{aligned}$$

Reversing the gradient and the expectation

Fact:

$$\nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) = q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}).$$

With this,

$$\begin{aligned}
\nabla_{\nu} \mathcal{L} &= \nabla_{\nu} \int q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\
&= \int \nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\
&= \int q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\
&= \mathbb{E}_{q(\mathbf{z}; \boldsymbol{\nu})} [\nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu})]
\end{aligned}$$

Reversing the gradient and the expectation

Fact:

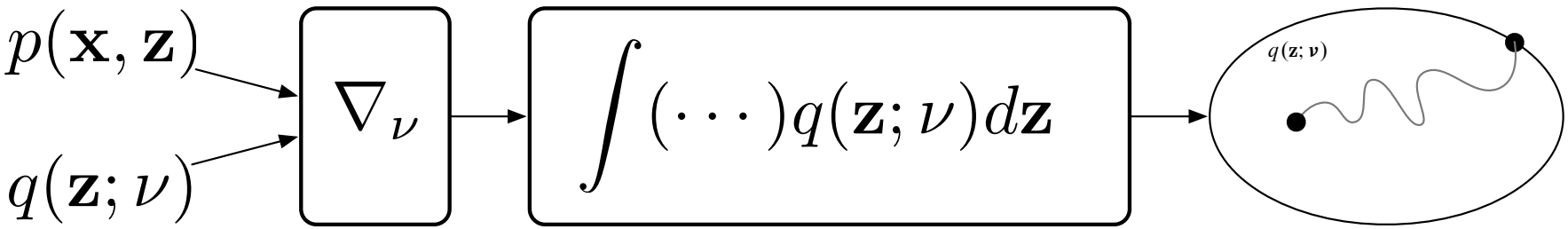
$$\nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) = q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}).$$

With this,

$$\begin{aligned}
\nabla_{\nu} \mathcal{L} &= \nabla_{\nu} \int q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\
&= \int \nabla_{\nu} q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\
&= \int q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + q(\mathbf{z}; \boldsymbol{\nu}) \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu}) d\mathbf{z} \\
&= \mathbb{E}_{q(\mathbf{z}; \boldsymbol{\nu})} [\nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu}) g(\mathbf{z}, \boldsymbol{\nu}) + \nabla_{\nu} g(\mathbf{z}, \boldsymbol{\nu})]
\end{aligned}$$

We have written the gradient as an expectation.

Black box variational inference



- Derive the score gradient
- Derive the reparameterization gradient

The score gradient

- The black-box gradient is

$$\nabla_{\boldsymbol{\nu}} \mathscr{L} = \mathbb{E}_{q(\mathbf{z};\boldsymbol{\nu})}[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu}) g(\mathbf{z},\boldsymbol{\nu}) + \nabla_{\boldsymbol{\nu}} g(z,\boldsymbol{\nu})]$$

The score gradient

- The black-box gradient is

$$\nabla_{\boldsymbol{\nu}} \mathscr{L} = \mathbb{E}_{q(\mathbf{z};\boldsymbol{\nu})}[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu}) g(\mathbf{z},\boldsymbol{\nu}) + \nabla_{\boldsymbol{\nu}} g(z,\boldsymbol{\nu})]$$

- Simplify the second term

$$\mathbb{E}_q[\nabla_{\boldsymbol{\nu}} g(\mathbf{z},\boldsymbol{\nu})] = \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu})] = 0$$

The score gradient

- The black-box gradient is

$$\nabla_{\boldsymbol{\nu}} \mathcal{L} = \mathbb{E}_{q(\mathbf{z};\boldsymbol{\nu})}[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu}) g(\mathbf{z},\boldsymbol{\nu}) + \nabla_{\boldsymbol{\nu}} g(z,\boldsymbol{\nu})]$$

- Simplify the second term

$$\mathbb{E}_q[\nabla_{\boldsymbol{\nu}} g(\mathbf{z},\boldsymbol{\nu})] = \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu})] = 0$$

- This gives the score gradient

$$\nabla_{\boldsymbol{\nu}} \mathcal{L} = \mathbb{E}_{q(\mathbf{z};\boldsymbol{\nu})}[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu})(\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\boldsymbol{\nu}))]$$

The reparameterization gradient

- Assume that we can express the variational distribution with a transformation, where

$$\begin{aligned}\boldsymbol{\epsilon} &\sim s(\boldsymbol{\epsilon}) \\ \mathbf{z} &= t(\boldsymbol{\epsilon}, \boldsymbol{\nu}) \\ &\rightarrow \mathbf{z} \sim q(\mathbf{z}; \boldsymbol{\nu})\end{aligned}$$

- For example,

$$\begin{aligned}\epsilon &\sim \text{Normal}(0, 1) \\ z &= \epsilon\sigma + \mu \\ &\rightarrow z \sim \text{Normal}(\mu, \sigma^2)\end{aligned}$$

- Also assume $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z})$ are differentiable with respect to $\mathbf{z}$

The reparameterization gradient

- The black box gradient is

$$\nabla_{\boldsymbol{\nu}} \mathscr{L} = \mathbb{E}_{q(\mathbf{z};\boldsymbol{\nu})}[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu}) g(\mathbf{z},\boldsymbol{\nu}) + \nabla_{\boldsymbol{\nu}} g(\mathbf{z},\boldsymbol{\nu})]$$

The reparameterization gradient

- The black box gradient is

$$\nabla_{\boldsymbol{\nu}} \mathcal{L} = \mathbb{E}_{q(\mathbf{z};\boldsymbol{\nu})}[\nabla_{\boldsymbol{\nu}} \log q(\mathbf{z};\boldsymbol{\nu}) g(\mathbf{z},\boldsymbol{\nu}) + \nabla_{\boldsymbol{\nu}} g(\mathbf{z},\boldsymbol{\nu})]$$

- Rewrite using using $\mathbf{z} = t(\boldsymbol{\epsilon},\boldsymbol{\nu})$,

$$\nabla_{\boldsymbol{\nu}} \mathcal{L} = \mathbb{E}_{s(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\nu}} \log s(\boldsymbol{\epsilon}) g(t(\boldsymbol{\epsilon},\boldsymbol{\nu}),\boldsymbol{\nu}) + \nabla_{\boldsymbol{\nu}} g(t(\boldsymbol{\epsilon},\boldsymbol{\nu}),\boldsymbol{\nu})]$$

The reparameterization gradient

- The black box gradient is

$$\nabla_{\nu} \mathcal{L} = \mathbb{E}_{q(\mathbf{z};\nu)}[\nabla_{\nu} \log q(\mathbf{z};\nu) g(\mathbf{z},\nu) + \nabla_{\nu} g(\mathbf{z},\nu)]$$

- Rewrite using using $\mathbf{z} = t(\epsilon, \nu)$,

$$\nabla_{\nu} \mathcal{L} = \mathbb{E}_{s(\epsilon)}[\nabla_{\nu} \log s(\epsilon) g(t(\epsilon,\nu),\nu) + \nabla_{\nu} g(t(\epsilon,\nu),\nu)]$$

- Note that $\nabla_{\nu} \log s(\epsilon) = 0$. Now use the chain rule:

$$\begin{aligned}
\nabla_{\nu} \mathcal{L} &= \mathbb{E}_{s(\epsilon)}[\nabla_{\nu} g(t(\epsilon,\nu),\nu)] \\
&= \mathbb{E}_{s(\epsilon)}[\nabla_{\mathbf{z}}[\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\nu)] \nabla_{\nu} t(\epsilon,\nu) - \nabla_{\nu} \log q(\mathbf{z};\nu)] \\
&= \mathbb{E}_{s(\epsilon)}[\nabla_{\mathbf{z}}[\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z};\nu)] \nabla_{\nu} t(\epsilon,\nu)]
\end{aligned}$$

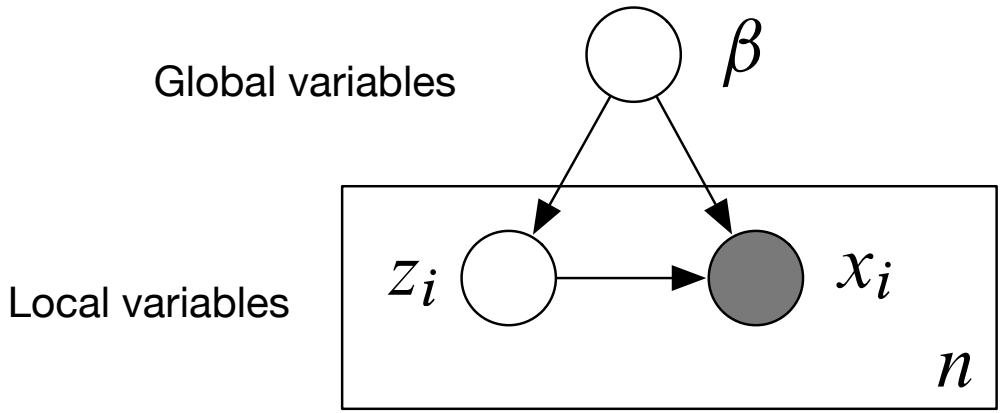
This is the reparameterization gradient.

[Glasserman 1991; Fu 2006; Kingma+ 2014; Rezende+ 2014; Titsias+ 2014]

Black box variational inference

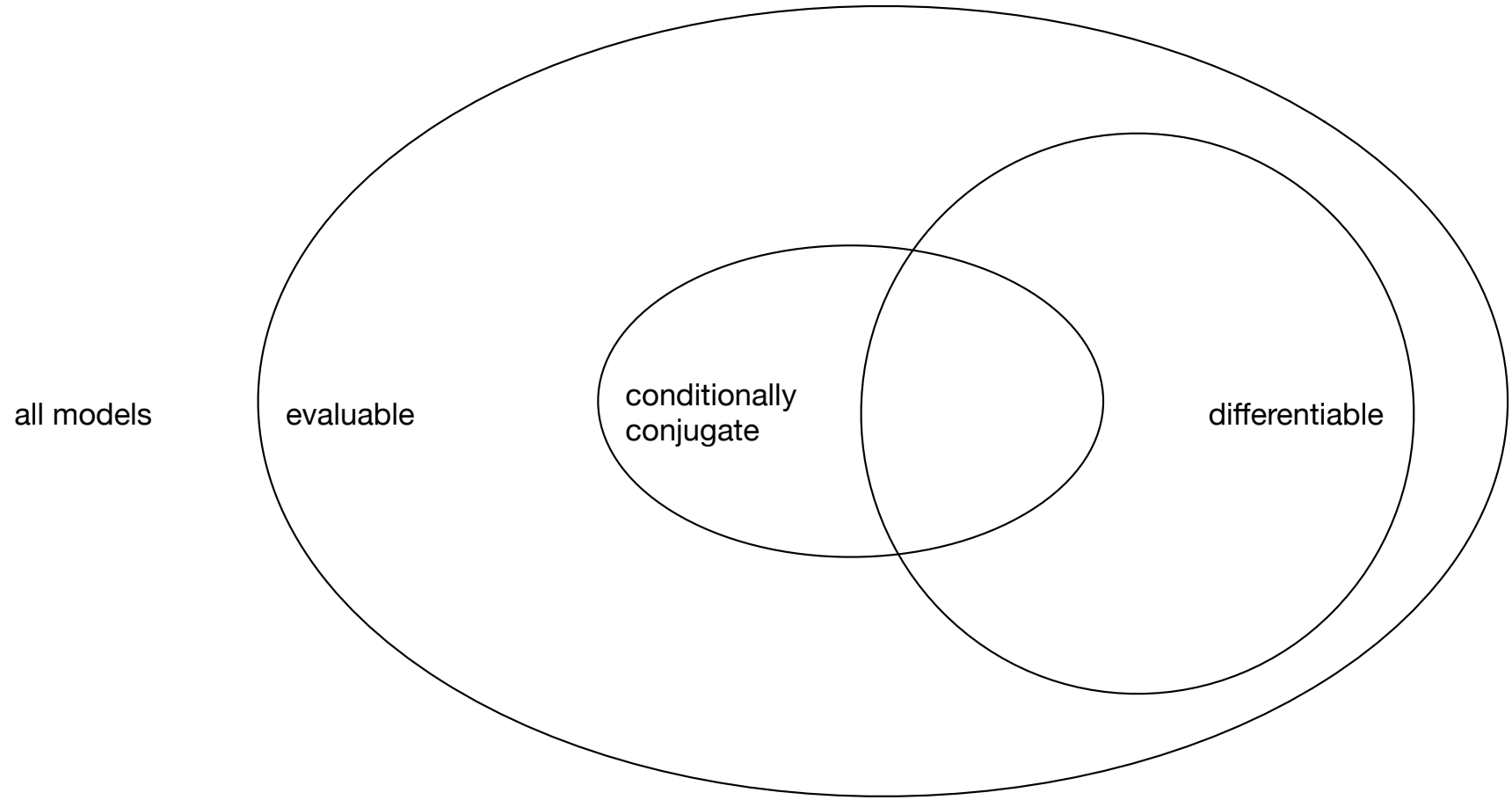
- BBVI with the score gradient
- BBVI with the reparameterization gradient
- Probabilistic programming and autodifferentiation VI
- How to derive BBVI

Nonconjugate models



$$p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^{n} p(z_i, x_i \mid \beta)$$

- Nonlinear time series models
- Deep latent Gaussian models
- Models with attention
- Generalized linear models
- Stochastic volatility models
- Discrete choice models
- Bayesian neural networks
- Deep exponential families
- Correlated topic models
- Sigmoid belief networks

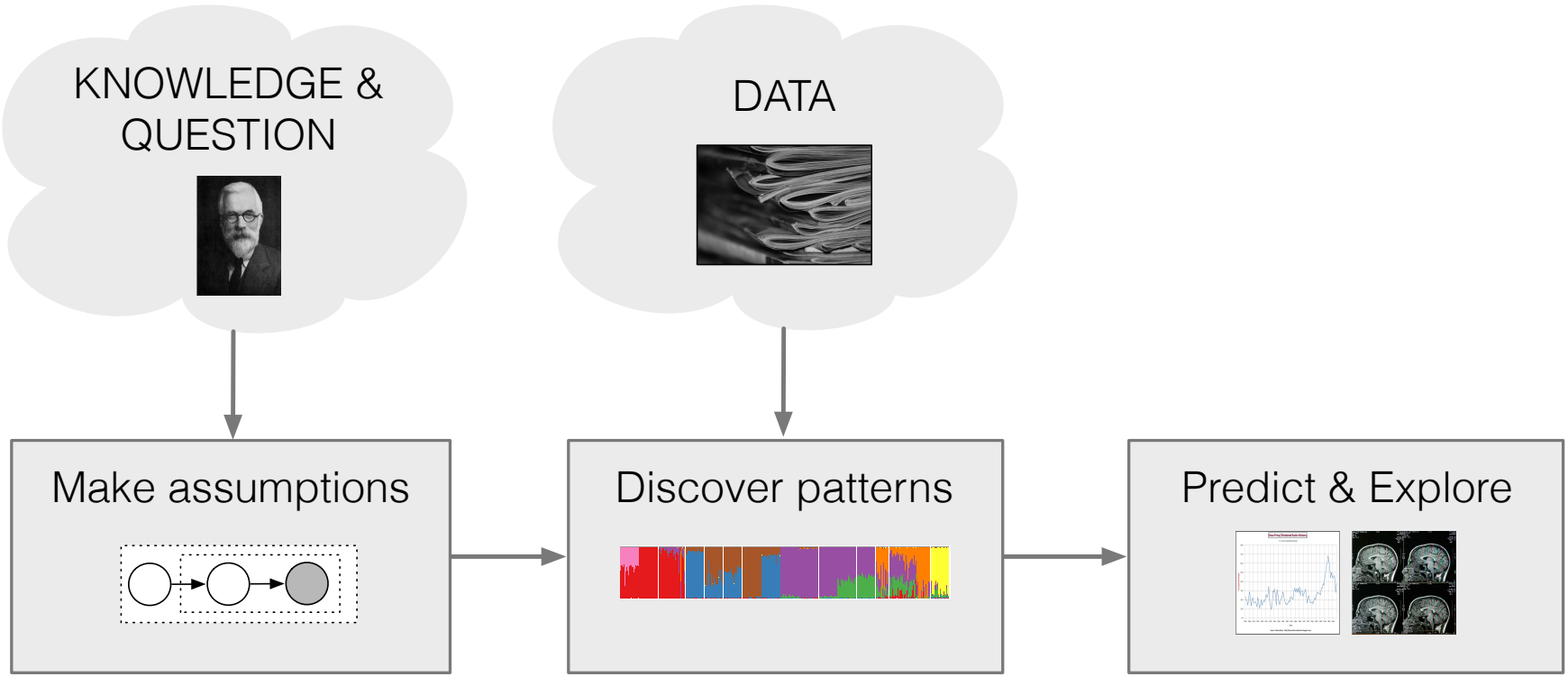

all models
evaluable
conditionally
conjugate
differentiable

A Tour of Variational Inference (with one picture)

PROBABILISTIC MACHINE LEARNING

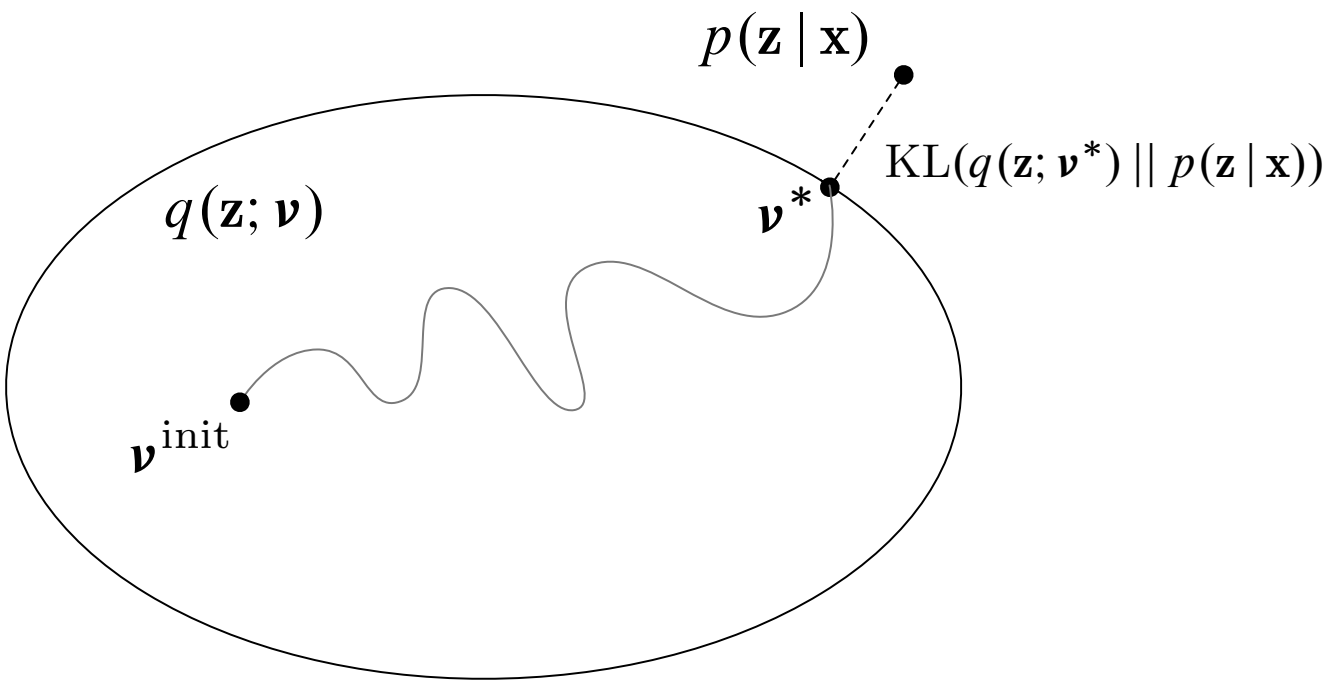
- ML methods that *connect domain knowledge to data*.
- Provides a computational methodology for scalable modeling
- Goal: A methodology that is *expressive, scalable, easy to develop*

The probabilistic pipeline



- **Posterior inference** is the key algorithmic problem.
- Answers the question: What does this model say about this data?
- VI provides **General** and **scalable** approaches to posterior inference

Stochastic optimization makes VI better

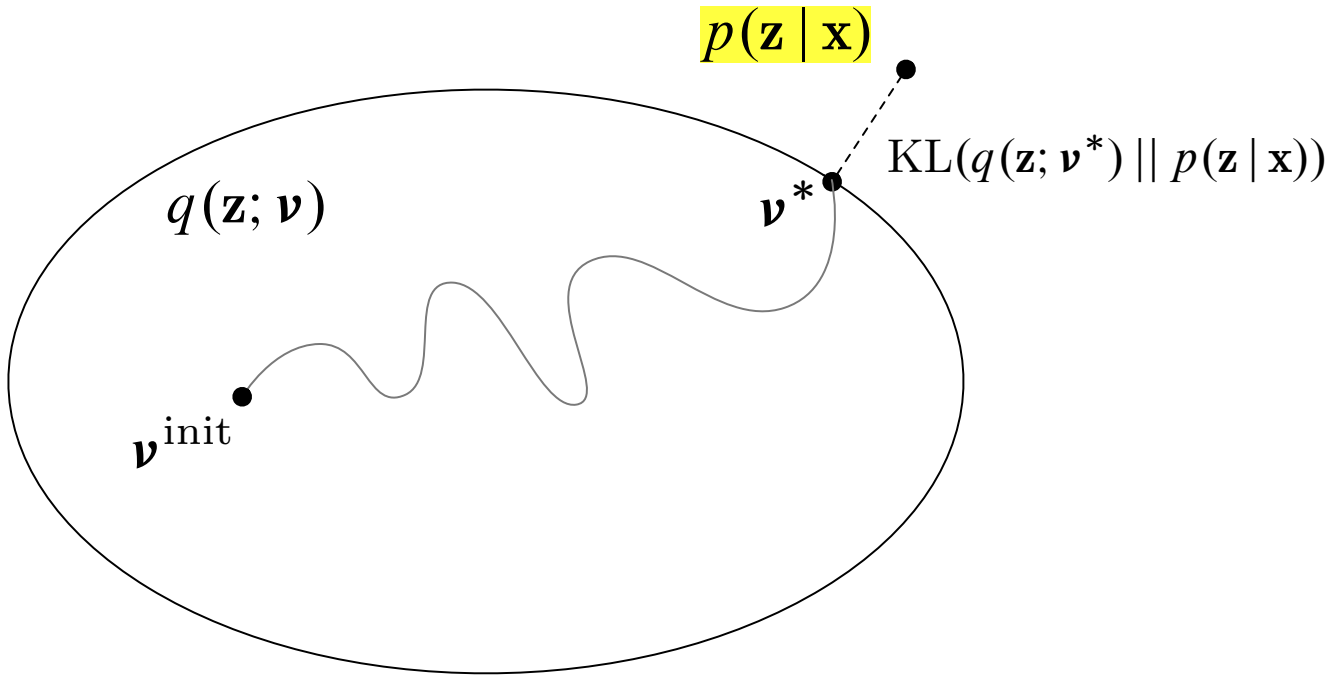


- **Stochastic VI** scales up VI to massive data.
- **Black box VI** generalizes VI to a wide class of models.

What we learned about

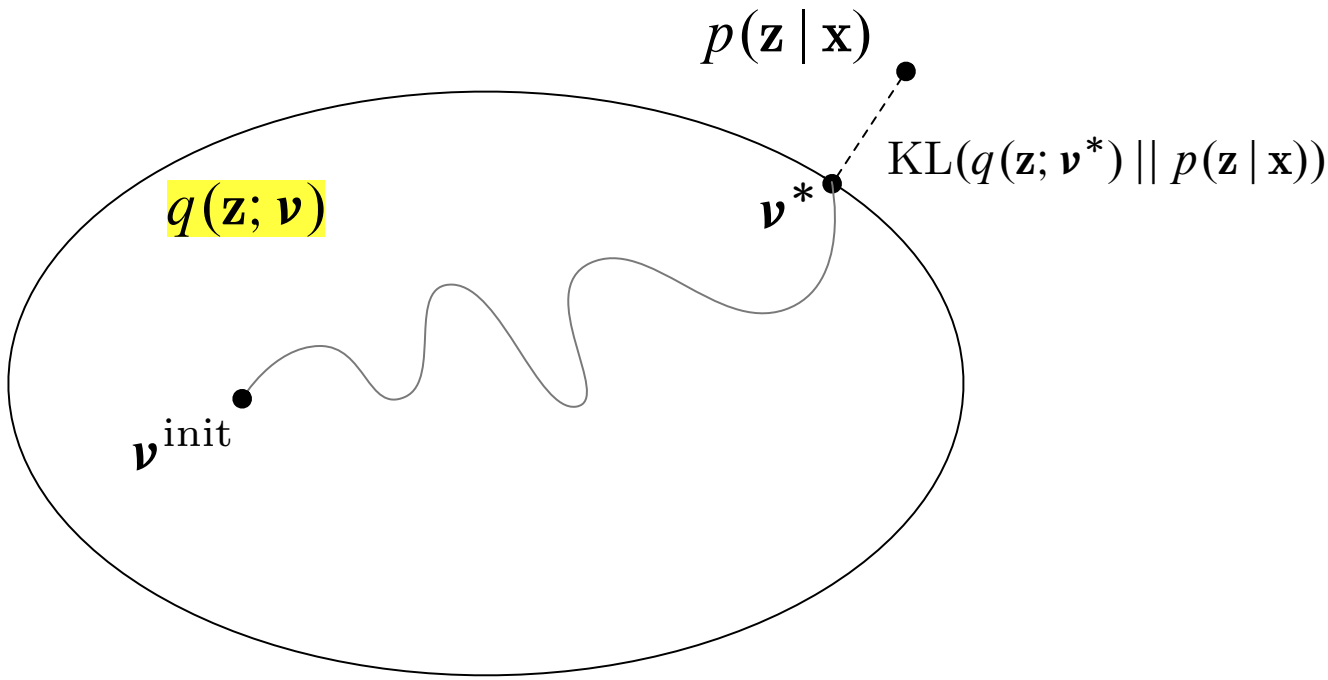
- The basics of variational inference (VI)
  - Mean-field variational inference
  - Coordinate ascent optimization for VI
- Stochastic variational inference for massive data
- Black box variational inference
  - Score gradients
  - Reparameterization gradients
  - Amortized variational families, the variational autoencoder
  - Probabilistic programming
- Models, along the way
  - Latent Dirichlet allocation and topic models
  - Deep exponential families
  - Embedding models of consumer behavior
  - Deep generative models

The class of models



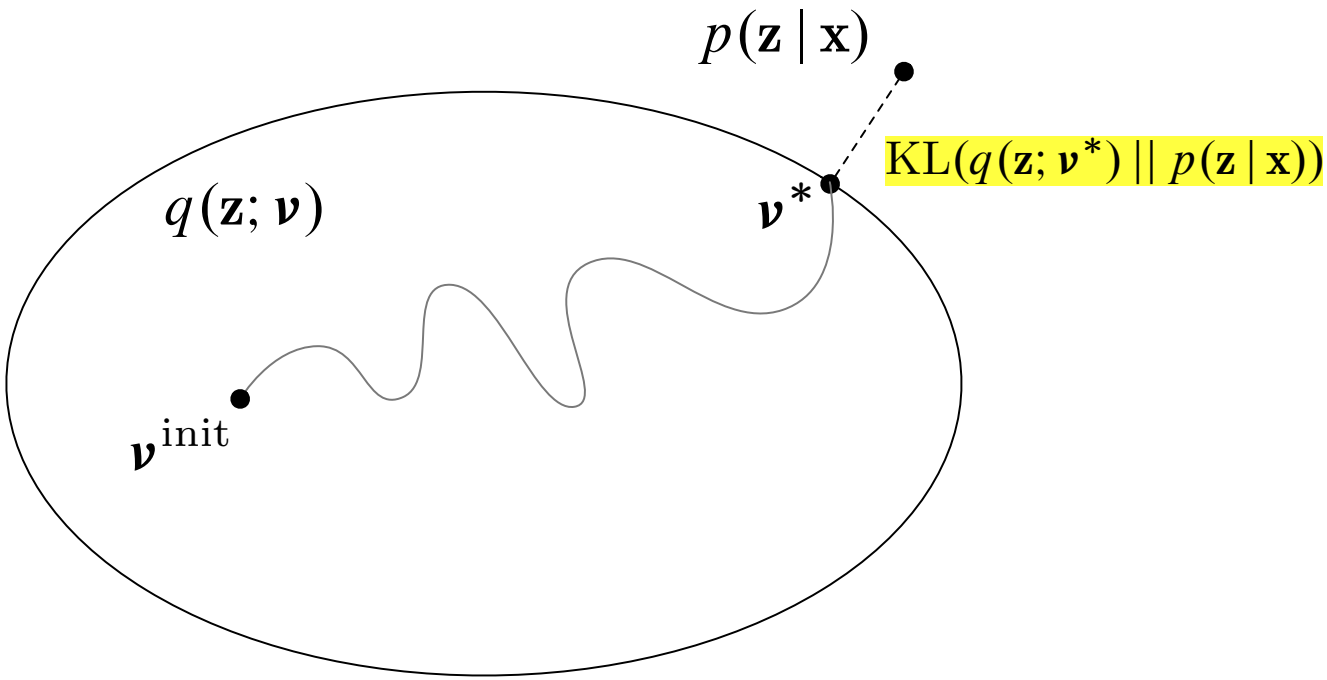
- Conditionally conjugate [Gharamani and Beal 2001; Hoffman+ 2013]
- Not ↑, but can differentiate the log likelihood [Kucukelbir+ 2015]
- Not ↑, but can calculate the log likelihood [Ranganath+ 2014]
- Not ↑, but can sample from the model [Ranganath+ 2017]

The family of variational approximations



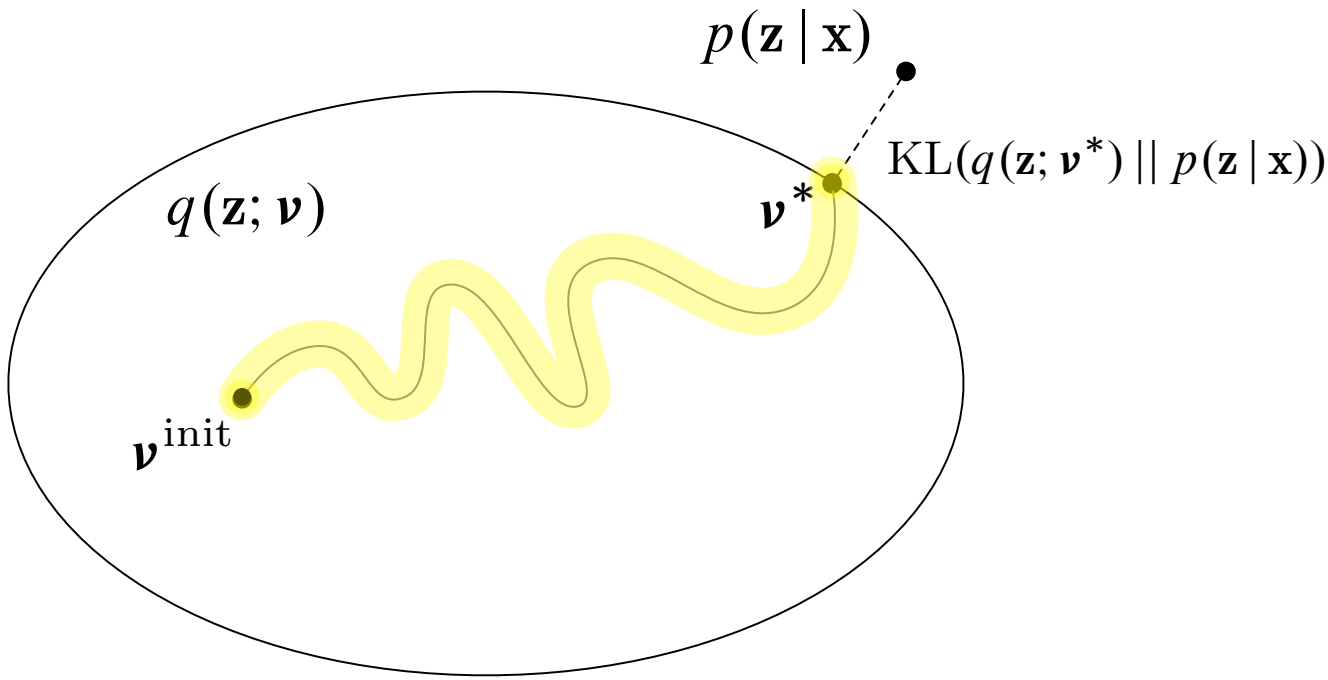
- Structured variational inference [Saul and Jordan 1996; Hoffman and Blei 2015]
- Variational models [Lawrence 2001; Ranganath+ 2015; Tran+ 2015]
- Amortized inference [Kingma and Welling 2014; Rezende+ 2014]
- Sequential Monte Carlo [Naesseth+ 2018; Maddison+ 2017; Le+ 2017]

The distance function



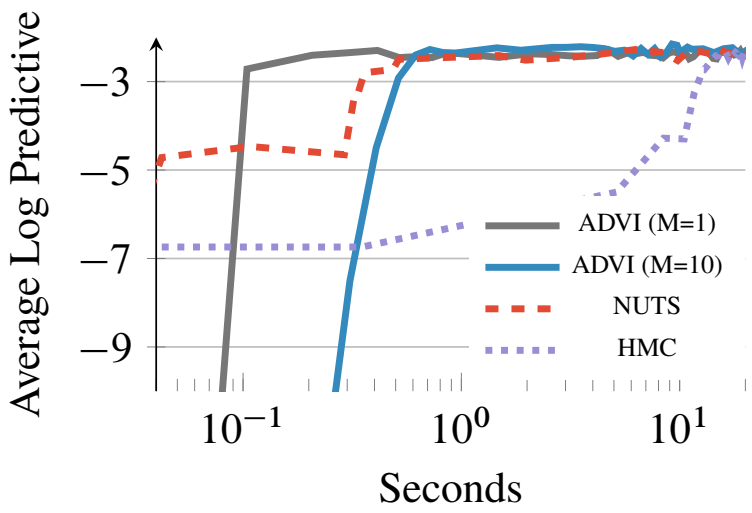
- Expectation propagation [Minka 2001]
- Belief propagation [Yedidia 2001]
- Operator variational inference [Ranganath+ 2016]
- χ-variational inference [Dieng+ 2017]

The algorithm

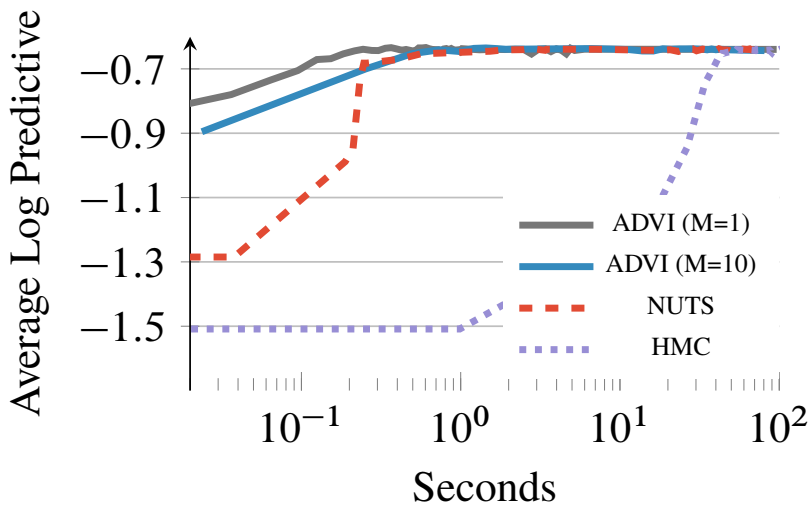


- SVI and structured SVI [Hoffman+ 2013; Hoffman and Blei 2015]
- Proximity VI [Altosaar+ 2018]
- SGD as VI [Mandt+ 2017]
- Adaptive rates, averaged and biased gradients, etc. [Many papers]

Should I be skeptical about variational inference?



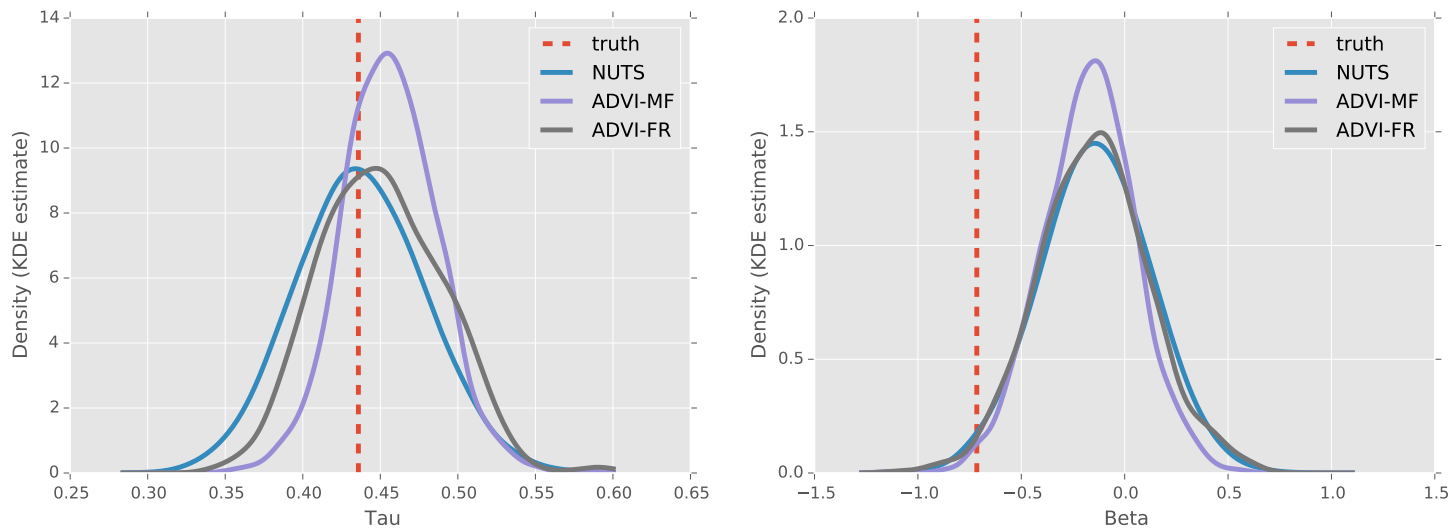
(a) Linear Regression with ARD



(b) Hierarchical Logistic Regression

- **MCMC enjoys theoretical guarantees.**
- But they usually get to the same place. [Kucukelbir+ 2016]
- We need more theory about variational inference.

Should I be skeptical about variational inference?



- **Variational inference underestimates the variance of the posterior.**
- Relaxing the mean-field assumption can help.
- Here: A Poisson GLM [Giordano+ 2015]

Some open problems in VI

- **Theory**
  MCMC has been widely analyzed and studied; VI is less explored.

- **Optimization**
  Can we find better local optima? Can we accelerate convergence?

- **Alternative divergences**
  KL is chosen for convenience; can we use other divergences?

- **Better approximations**
  VI underestimates posterior variance. Can we do better?

- D. Blei, A. Kucukelbir, J. McAuliffe. **Variational inference: A review for statisticians**. Journal of American Statistical Association, 2017.

- M. Hoffman, D. Blei, C. Wang, J. Paisley. **Stochastic variational inference**. Journal of Machine Learning Research, 2013.

- R. Ranganath, S. Gerrish, D. Blei. **Black box variational inference**. Artificial Intelligence and Statistics, 2014.

- A. Kucukelbir, D. Tran, R. Ranganath, A. Gelman, D. Blei. **Automatic differentiation variational inference**. Journal of Machine Learning Research, 2017.

- R. Ranganath, L. Tang, L. Charlin, D. Blei. **Deep exponential families**. Artificial Intelligence and Statistics, 2015.

- F. Ruiz, S. Athey, D. Blei. **Shopper: A probabilistic model of consumer choice with substitutes and complements.** arXiv:1711.03560, 2017.

VAMOS ARGENTINA!!!!!