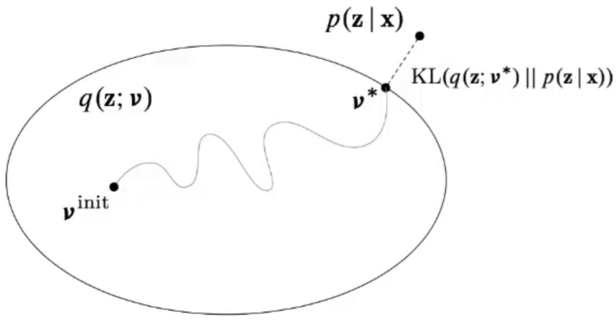
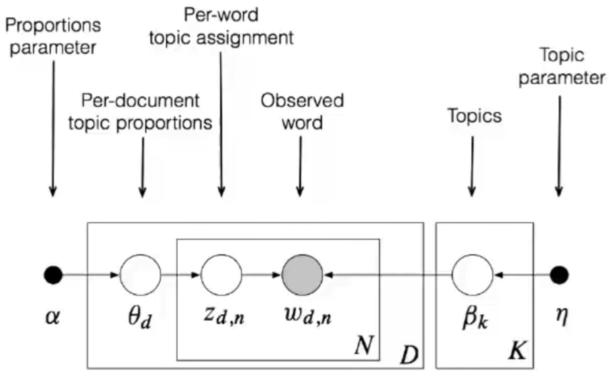
Reference: [Variational Inference: Foundations and Modern Methods - David Blei, Shakir Mohamed] (NIPS 2016 tutorial)

Part 1: Background

- **Probabilistic Pipeline**
  - (Assumptions -> Model, Data) -> Discover Patterns -> Predict & Explore
- **Probabilistic Machine Learning**
  - probabilistic model: p(z, x)
    - z - hidden. variables
    - x - observed variables
  - inference about unknowns through the **posterior**: $p(z|x) = \frac{p(z,x)}{p(x)}$
    - For most interesting models, the denominator is intractable
    - Hence **approximate posterior inference** is required
      - MCMC - forms a Markov Chain whose stationary distribution is $p(z|x)$
      - Variational Inference
- **Variational Inference**
  - 

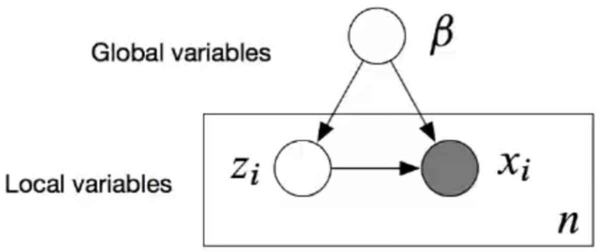
  - VI turns **inference into optimization**.
  - Posit a **variational family** of distributions over the latent variables, $q(\mathbf{z}; \boldsymbol{v})$
  - Fit the **variational parameters** ν to be close (in KL) to the exact posterior.
    - There are alternative divergences, which connect to algorithms like EP, BP, and others.
- Posterior Predictive Distributions
- Modern VI: probabilistic programming, RL, NNs, Convex optimization, Bayesian Statistics
- VI + Stochastic Optimisation
  - scale up VI to massive data
  - enable VI on a wide class of difficult models
  - enable VI with elaborate and flexible families of approximations

Part 2: Mean-field VI and Stochastic VI

- Topic models: Use posterior inference to discover the hidden thematic structure in a large collection of documents. Eg. LDA
- LDA
  - 

- idea:
  - 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
- A **Mixed Membership model** for which the Z is intractable.
- $p(\beta, \boldsymbol{\theta}, \mathbf{z} \mid \mathbf{w}) = \frac{p(\beta, \boldsymbol{\theta}, \mathbf{z}, \mathbf{w})}{\int_\beta \int_{\boldsymbol{\theta}} \sum_{\mathbf{z}} p(\beta, \boldsymbol{\theta}, \mathbf{z}, \mathbf{w})}$
- The denominator, $p(w)$ is intractable and requires approximate inference.
  Define the generic class of conditionally conjugate models
  Derive classical mean-field VI
  Derive stochastic VI, which scales to massive data

Generic Class of Conditionally Conjugate Models

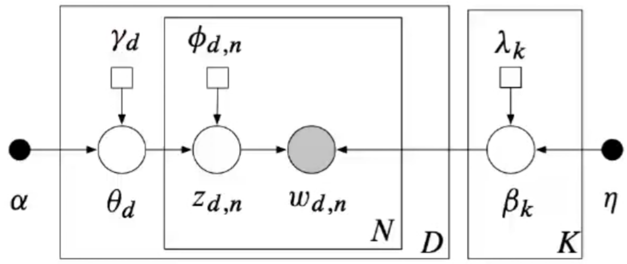
- 

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

- 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 $p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^{n} p\left(z_i, x_i \mid \beta\right)$
- 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,
  - $$p\left(z_i \mid \beta, x_i\right) = h\left(z_i\right) \exp\left\{\eta_\ell\left(\beta, x_i\right)^\top z_i - a\left(\eta_\ell\left(\beta, x_i\right)\right)\right\}$$
    $$p(\beta \mid \mathbf{z}, \mathbf{x}) = h(\beta) \exp\left\{\eta_g(\mathbf{z}, \mathbf{x})^\top \beta - a\left(\eta_g(\mathbf{z}, \mathbf{x})\right)\right\}$$
- The global parameter comes from conjugacy and has a particular form: [Bernardo and Smith, 1994]
  - $\eta_g(\mathbf{z}, \mathbf{x}) = \alpha + \sum_{i=1}^{n} t\left(z_i, x_i\right)$
  - where α is a hyperparameter and $t(\cdot)$ are sufficient statistics for $[z_i, x_i]$.
- Examples:
  - Bayesian mixture models
  - Time series models
  - Factorial models
  - Matrix Factorization
  - Mixed-membership models (LDA etc.)
  - etc.
- **Evidence Lower Bound**
  - $\mathscr{L}(\boldsymbol{v}) = \mathbb{E}_{\beta, z \sim q}[\log p(\beta, \mathbf{z}, \mathbf{x})] - \mathbb{E}_{\beta, z \sim q}[\log q(\beta, \mathbf{z}; \boldsymbol{v})]$
    - FIrst term is *expected likelihood* and the second is *entropy*.
  - KL is intractable as it requires knowing the posterior itself
  - VI optimizes the evidence lower bound (ELBO) instead which 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 (entropy of q) encourages $q(\cdot)$ to be diffuse.
  - *Caveat*: The ELBO is not convex.
    - => Find a local optimum
- **Mean-Field Family**
  -

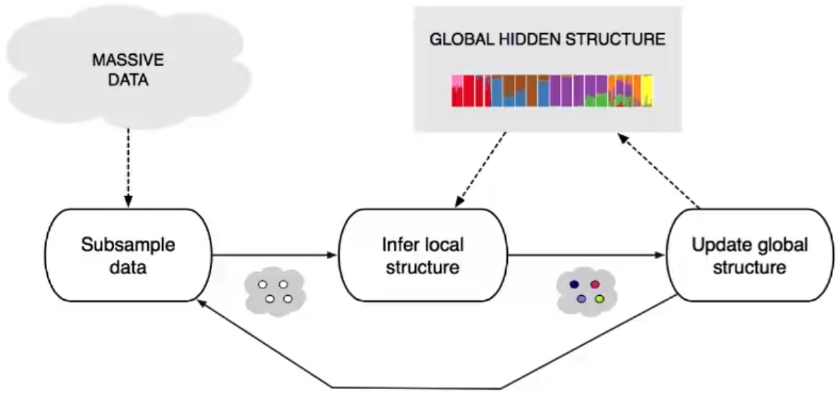
- A form of $q(\beta, \mathbf{z})$.
- **Fully factorized**: All latent variables are independent and governed by their on variational parameters.
  - $q(\beta, \mathbf{z}; \lambda, \phi) = q(\beta; \lambda) \prod_{i=1}^{n} q\left(z_i; \phi_i\right)$
- Each factor is the same family as the model's complete conditional,
  - $$\begin{aligned} p(\beta \mid \mathbf{z}, \mathbf{x}) &= h(\beta) \exp\left\{\eta_g(\mathbf{z}, \mathbf{x})^{\top} \beta - a\left(\eta_g(\mathbf{z}, \mathbf{x})\right)\right\} \\ q(\beta; \lambda) &= h(\beta) \exp\left\{\lambda^{\top} \beta - a(\lambda)\right\} \end{aligned}$$

Classical Mean Field VI

- Optimize the ELBO, $\mathscr{L}(\lambda, \boldsymbol{\phi}) = \mathbb{E}_q[\log p(\beta, \mathbf{z}, \mathbf{x})] - \mathbb{E}_q[\log q(\beta, \mathbf{z})]$
- **Traditional VI uses coordinate ascent** [Ghahramani and Beal, 2001]
  - $\lambda^* = \mathbb{E}_\phi\left[\eta_g(\mathbf{z}, \mathbf{x})\right]$
  - $\phi_i^* = \mathbb{E}_\lambda\left[\eta_\ell\left(\beta, x_i\right)\right]$
- Iteratively update each parameter, holding others fixed.
  - Notice the relationship to Gibbs sampling [Gelfand and Smith, 1990]
    - In Gibbs Sampling we iteratively sample from the distributions,
      - In VI we set it to the expectation
  - Caveat: The ELBO is not convex.
- **Mean Field VI 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
  - $q(\beta, \boldsymbol{\theta}, \mathbf{z}) = \prod_{k=1}^{K} q\left(\beta_k; \lambda_k\right) \prod_{d=1}^{D} q\left(\theta_d; \gamma_d\right) \prod_{n=1}^{N} q\left(z_{d,n}; \phi_{d,n}\right)$
-
- *Algorithm*
  - **Input**: data x, model $p(\beta, \mathbf{z}, \mathbf{x})$.
  - Initialize λ randomly.
  - repeat until the ELBO has converged:
    - for each data point i:
      - Set local parameter $\phi_i \leftarrow \mathbb{E}_\lambda\left[\eta_\ell\left(\beta, x_i\right)\right]$
    - Set global parameter $\lambda \leftarrow \alpha + \sum_{i=1}^{n} \mathbb{E}_{\phi_i}\left[t\left(Z_i, x_i\right)\right]$
- *Problem*: Classical VI is inefficient
  - Need to local computation for each data point, aggregate them to reestimate the global structure and repeat.
- *Solution*: Stochastic VI scales VI to massive data.

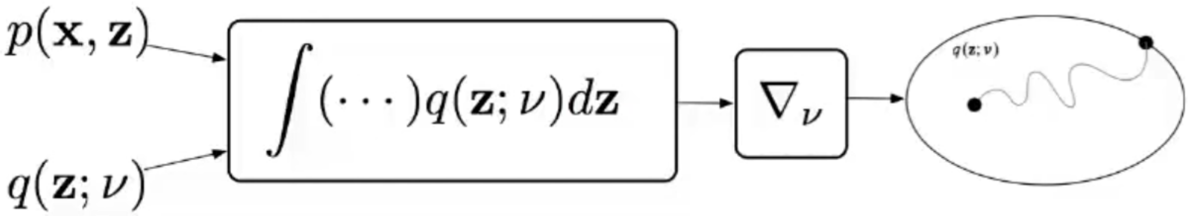
Stochastic VI



- **Stochastic Optimization**
  - With noisy gradients, update
    - $v_{t+1} = v_t + \rho_t \hat{\nabla}_v \mathscr{L}(v_t)$
  - Requires unbiased gradients, $\mathbb{E}\left[\hat{\nabla}_\nu \mathscr{L}(v)\right] = \nabla_v \mathscr{L}(v)$
  - Requires the step size sequence ρ_t follows the Robbins-Monro conditions
- **Stochastic VI**
  - The natural gradient of the ELBO [Amari, 1998; Sato, 2001]
    - $\nabla_\lambda^{\text{nat}} \mathscr{L}(\lambda) = \left(\alpha + \sum_{i=1}^n \mathbb{E}_{\phi_i^*}\left[t\left(Z_i, x_i\right)\right]\right) - \lambda$
    - second term is the sum of expectations of the sufficient statistics.
  - Construct a noisy natural gradient,
    - $$\begin{aligned} j &\sim \text{ Uniform }(1, \ldots, n) \\ \hat{\nabla}_\lambda^{\text{nat}} \mathscr{L}(\lambda) &= \alpha + n \mathbb{E}_{\phi_j^*}\left[t\left(Z_j, x_j\right)\right] - \lambda \end{aligned}$$
  - This is a good noisy gradient.
    - Its expectation is the exact gradient (unbiased).
    - It only depends on optimized parameters of one data point (cheap).
  - *Algorithm*:
    - Input: data x, model $p(\beta, \mathbf{z}, \mathbf{x})$.
    - Initialize λ randomly. Set ρ_t appropriately.
    - repeat until forever
      - Sample $j \sim \operatorname{Unif}(1, \ldots, n)$
      - Set local parameter $\phi \leftarrow \mathbb{E}_\lambda\left[\eta_\ell\left(\beta, x_j\right)\right]$
      - Set intermediate global parameter $\hat{\lambda} = \alpha + n \mathbb{E}_\phi\left[t\left(Z_j, x_j\right)\right]$
      - Set global parameter $\lambda = \left(1 - \rho_t\right) \lambda + \rho_t \hat{\lambda}$
  - Eg. LDA
    1. Sample a document
    2. Estimate the local variational parameters using the current topics
    3. Form intermediate topics from those local parameters
    4. Update topics as a weighted average of intermediate and current topics

Part 3: Stochastic gradients of the ELBO

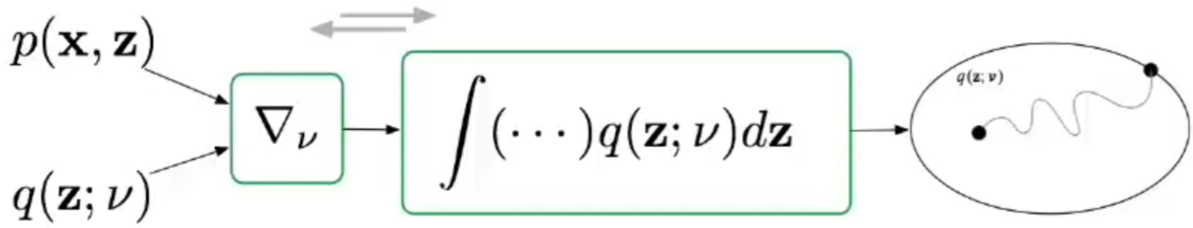
VI Recipe

- 

- Start with a model: $p(z, x)$
- Choose a variational approximation: $q(\mathbf{z}; \boldsymbol{v})$
- Write down the ELBO: $\mathscr{L}(\boldsymbol{v}) = \mathbb{E}_{q(\mathbf{z}; \boldsymbol{v})}[\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}; \boldsymbol{v})]$
- Take derivatives: $\nabla_v \mathscr{L}$
- Optimize: $v_{t+1} = v_t + \rho_t \nabla_v \mathscr{L}$

- Example: Bayesian Logistic Regression
    - Data pairs y_i, x_i
    - x_i are covariates
    - y_i are label
    - z is the regression coefficient
    - Generative process
        - $$\begin{aligned} p(z) &\sim N(0,1) \\ p\left(y_i \mid x_i, z\right) &\sim \operatorname{Bernoulli}\left(\sigma\left(z x_i\right)\right) \end{aligned}$$
    - VI for Bayesian LR
        - Assume:
            - We have one data point (y, x)
            - x is a scalar
            - The approximating family q is the normal; $\boldsymbol{v}=\left(\mu, \sigma^2\right)$
        - The ELBO is
            - $$\begin{aligned} \mathscr{L}\left(\mu, \sigma^2\right) &= \mathbb{E}_q[\log p(z)+\log p(y \mid x, z)-\log q(z)] \\ &= \mathbb{E}_q[\log p(z)-\log q(z)+\log p(y \mid x, z)] \\ &= -\frac{1}{2}\left(\mu^2+\sigma^2\right)+\frac{1}{2} \log \sigma^2+\mathbb{E}_q[\log p(y \mid x, z)]+C \\ &= -\frac{1}{2}\left(\mu^2+\sigma^2\right)+\frac{1}{2} \log \sigma^2+\mathbb{E}_q[y x z-\log (1+\exp (x z))] \\ &= -\frac{1}{2}\left(\mu^2+\sigma^2\right)+\frac{1}{2} \log \sigma^2+y x \mu-\mathbb{E}_q[\log (1+\exp (x z))] \end{aligned}$$
            - We are stuck.
                - We cannot analytically take that expectation.
                - The expectation hides the objectives dependence on the variational parameters. This makes it hard to directly optimize.
    - Want a blackbox VI algorithm that works for non-Conjugate models as well.

New Blackbox VI recipe

- 

- Define $g(\mathbf{z}, \boldsymbol{v})=\log p(\mathbf{x}, \mathbf{z})-\log q(\mathbf{z} ; \boldsymbol{v})$
- $$\begin{aligned} \nabla_v \mathscr{L} &= \nabla_v \int q(\mathbf{z} ; \boldsymbol{v}) g(\mathbf{z}, \boldsymbol{v}) d \mathbf{z} \\ &= \int \nabla_v q(\mathbf{z} ; \boldsymbol{v}) g(\mathbf{z}, \boldsymbol{v})+q(\mathbf{z} ; \boldsymbol{v}) \nabla_v g(\mathbf{z}, \boldsymbol{v}) d \mathbf{z} \\ &= \int q(\mathbf{z} ; \boldsymbol{v}) \nabla_v \log q(\mathbf{z} ; \boldsymbol{v}) g(\mathbf{z}, \boldsymbol{v})+q(\mathbf{z} ; \boldsymbol{v}) \nabla_{\boldsymbol{v}} g(\mathbf{z}, \boldsymbol{v}) d \mathbf{z} \\ &= \mathbb{E}_{q(\mathbf{z} ; \boldsymbol{v})}\left[\nabla_{\boldsymbol{v}} \log q(\mathbf{z} ; \boldsymbol{v}) g(\mathbf{z}, \boldsymbol{v})+\nabla_v g(\mathbf{z}, \boldsymbol{v})\right] \end{aligned}$$

Score-Function Gradients

- Simplify $\nabla_\nu \mathscr{L}$:
    - $\mathbb{E}_q\left[\nabla_\nu g(\mathbf{z}, \boldsymbol{v})\right]=\mathbb{E}_q\left[\nabla_\nu \log q(\mathbf{z} ; \boldsymbol{v})\right]=0$
        - [score function has expectation zero]
- Gives the gradient:
    - $\nabla_v \mathscr{L}=\mathbb{E}_{q(\mathbf{z} ; \boldsymbol{v})}\left[\nabla_\nu \log q(\mathbf{z} ; \boldsymbol{v})(\log p(\mathbf{x}, \mathbf{z})-\log q(\mathbf{z} ; \boldsymbol{v}))\right]$
    - Called **Score Function Estimator** or **likelihood ratio** or **REINFORCE gradients**
- **Noisy Unbiased Gradients with Monte-Carlo**
    - $\frac{1}{S} \sum_{s=1}^S \nabla_v \log q\left(\mathbf{z}_s ; \boldsymbol{v}\right)\left(\log p\left(\mathbf{x}, \mathbf{z}_s\right)-\log q\left(\mathbf{z}_s ; \boldsymbol{v}\right)\right)$
        - where $\mathbf{z}_s \sim q(\mathbf{z} ; \boldsymbol{v})$
    - Requirements for Inference i.e. to compute the noisy gradient of the ELBO we need
        - Sampling from $q(\mathbf{z})$
        - Evaluating $\nabla_\nu \log q(\mathbf{z} ; \boldsymbol{v})$
        - Evaluating $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z})$

- Nothing model-specific hence black-box satisfied
- *Problem*: Sampling rare values can lead to high scores and hence high variance
- *Solution*: *Control Variates*
  - Replace with f with $\hat{f}$ where $\mathbb{E}[\hat{f}(z)] = \mathbb{E}[f(z)]$.
  - General such class: $\hat{f}(z) \triangleq f(z) - a(h(z) - \mathbb{E}[h(z)])$
    - h is a function of our choice
    - a is chosen to minimize the variance
    - Good h have high correlation with the original function f
  - For VI, need h with known q expectation:
    - Set $h(z) = \nabla_v \log q(\mathrm{z}; \boldsymbol{v})$
    - Simple as $\mathbb{E}_q\left[\nabla_\nu \log q(\mathbf{z}; \boldsymbol{v})\right] = 0$ for any q

Pathwise Gradients

- Additional assumption that aren't very restrictive and allow faster or more efficient inference.
  - $\mathbf{z} = t(\epsilon, v)$ for $\epsilon \sim s(\epsilon)$ implies $\mathbf{z} \sim q(\mathbf{z}; v)$
    - Starting with noise that comes from distribution independent of ν, transform it using a function that depends on ν so that the resulting random variable $\mathbf{z}$ has distribution $q(\mathbf{z}; v)$
      $$\epsilon \sim \mathrm{Normal}(0, 1)$$
    - *Example*: $z = \epsilon\sigma + \mu$
      $$\rightarrow z \sim \mathrm{Normal}\left(\mu, \sigma^2\right)$$
  - $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z})$ are differentiable with respect to $\mathbf{z}$
- **Pathwise Estimator**
  - Rewrite $\nabla_\nu \mathscr{L}$ using using $\mathbf{z} = t(\boldsymbol{\epsilon}, \boldsymbol{v})$
    - $\nabla_\nu \mathscr{L} = \mathbb{E}_{s(\epsilon)}\left[\nabla_\nu \log s(\epsilon) g(t(\epsilon, v), v) + \nabla_v g(t(\epsilon, v), v)\right]$
    - Now the first term is zero as $\nabla_\nu \log s(\epsilon) = 0$.
  - Simplify:
    -
    - $$\begin{aligned} \nabla \mathscr{L}(v) &= \mathbb{E}_{s(\epsilon)}\left[\nabla_v g(t(\epsilon, v), v)\right] \\ &= \mathbb{E}_{s(\epsilon)}\left[\nabla_{\mathbf{z}}[\log p(\mathbf{x}, \mathbf{z}) \log q(\mathbf{z}; \boldsymbol{v})] \nabla_v t(\epsilon, v) - \nabla_v \log q(\mathbf{z}; \boldsymbol{v})\right] \\ &= \mathbb{E}_{s(\epsilon)}\left[\nabla_{\mathbf{z}}[\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}; \boldsymbol{v})] \nabla_v t(\boldsymbol{\epsilon}, \boldsymbol{v})\right] \end{aligned}$$
      - This again uses $\mathbb{E}_q\left[\nabla_\nu \log q(\mathbf{z}; \boldsymbol{v})\right] = 0$
  - Also known as the **reparameterization gradient**.
  - **Variance: Pathwise > Score function with control variate > Score Function**

Amortized Inference

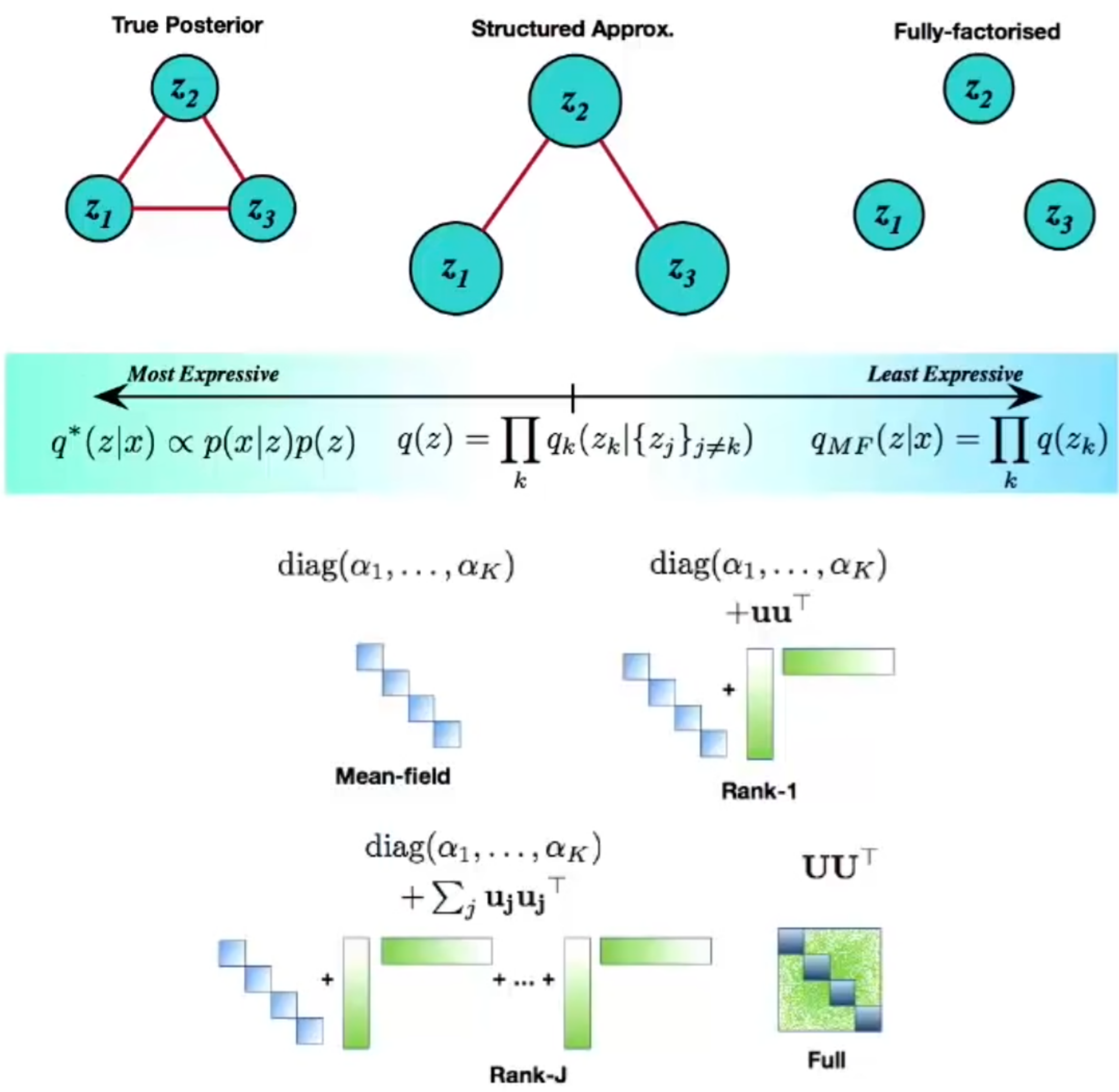
- *SVI revisited*:
  - Input: data x, model $p(\beta, \mathbf{z}, \mathbf{x})$.
  - Initialize λ randomly. Set ρ_t appropriately.
  - repeat until forever
    - Sample $j \sim \mathrm{Unif}(1, \ldots, n)$
    - Set local parameter $\phi \leftarrow \mathbb{E}_\lambda\left[\eta_\ell\left(\beta, x_j\right)\right]$
    - Set intermediate global parameter $\hat{\lambda} = \alpha + n\mathbb{E}_\phi\left[t\left(Z_j, x_j\right)\right]$
    - Set global parameter $\lambda = \left(1 - \rho_t\right)\lambda + \rho_t\hat{\lambda}$
- *Problem*: The expectaitons are no longer tractable and require stochastic optimization. But that stochastic optimisation for each data point make it too slow.
- *Solution*: Learn a mapping f from x_i to ϕ_i
  - ELBO:
    - $\mathscr{L}\left(\lambda, \phi_{1\ldots n}\right) = \mathbb{E}_q[\log p(\beta, \mathbf{z}, \mathbf{x})] - \mathbb{E}_q\left[\log q(\beta; \lambda) + \sum_{i=1}^n q\left(z_i; \phi_i\right)\right]$
  - Amortizing the ELBO with inference network f :
    - $\mathscr{L}(\lambda, \theta) = \mathbb{E}_q[\log p(\beta, \mathbf{z}, \mathbf{x})] - \mathbb{E}_q\left[\log q(\beta; \lambda) + \sum_{i=1}^n q\left(z_i \mid x_i; \phi_i = f_\theta\left(x_i\right)\right)\right]$
- **Amortized SVI**
  - Input: data x, model $p(\beta, \mathbf{z}, \mathbf{x})$.
  - Initialize λ randomly. Set ρ_t appropriately.
  - repeat until forever
    - Sample $\beta \sim q(\beta; \lambda)$
    - Sample $j \sim \mathrm{Unif}(1, \ldots, n)$

        - Sample $z_j \sim q\left(z_j \mid x_j ; \phi_\theta\left(x_j\right)\right.$
        - Compute stochastic gradients
        - $\hat{\nabla}_\lambda \mathscr{L}=\nabla_\lambda \log q(\beta ; \lambda)\left(\log p(\beta)+n \log p\left(x_j, z_j \mid \beta\right)-\log q(\beta)\right)$
          $\hat{\nabla}_\theta \mathscr{L}=n \nabla_\theta \log q\left(z_j \mid x_j ; \theta\right)\left(\log p\left(x_j, z_j \mid \beta\right)-\log q\left(z_j \mid x_k ; \theta\right)\right)$
        - Update
            - $\lambda=\lambda+\rho_t \hat{\nabla}_\lambda$
            - $\theta=\theta+\rho_t \hat{\nabla}_\theta$
    - **Computational-Statistical tradeoff**: Amortized inference is faster but admits a smaller class of approximations whose size depends on the flixibility of f.

Rules of Thumb for a New Model

- If $\log p(\mathbf{x}, \mathbf{z})$ is $\mathbf{z}$ differentiable
    - Try out an approximation q that is reparameterizable
- If $\log p(\mathbf{x}, \mathbf{z})$ is not $\mathbf{z}$ differentiable
    - use score function estimator with control variates
    - Add further variance reductions based on experimental evidence
- General Advice:
    - Use coordinate specific learning rates (eg. RMSProp, AdaGrad)
    - Annealing + Tempering
    - Consider sampling across samples from q (embarassingly parallelable)

Part 4: Beyond the Mean-field

- 

- - $q_G(\mathbf{z}; \boldsymbol{v}) = \mathcal{N}(\mathbf{z} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$
- **Beyond Gaussian Approximations**
    - **Autoregressive distributions**:
        - $q_{AR}(\mathbf{z}; \boldsymbol{v}) = \prod_k q_k\left(z_k \mid z_{<k}; \boldsymbol{v}_k\right)$
        - Impose an ordering and non-linear dependency on all preceding variables.
        - Joint distribution is non-gaussian even though the conditionals are.
    - More structured Posteriors