

[Paper review 44]

Variational Inference ; A Review for Statisticians

(Blei, et.al , 2018)

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1. Abstract

core problem : **difficult-to-compute pdf**

This paper : review VARIATIONAL INFERENCE

- approximates via optimization
- step 1) posit a family of densities
- step 2) find the member of that family, closest to the target

2. Introduction

VI :faster & easier to scale to LARGE data

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

- latent variables : $\mathbf{z} = \mathbf{z}_{1:m}$
(help govern the distn of data)
- observation : $\mathbf{x} = \mathbf{x}_{1:n}$

Draw latent variable from prior $p(\mathbf{z})$

Relate them to observation, via likelihood $p(\mathbf{z} | \mathbf{x})$

MCMC

- step 1) construct ergodic Markov chain on \mathbf{z}
(whose stationary distn is posterior $p(\mathbf{z} | \mathbf{x})$)
- step 2) sample from the chain (= collect samples from stationary distn)
- step 3) approximate posterior with collected samples

VI is needed, when we need faster speed than MCMC

- when data sets are **large**
- when models are **complex**

Rather than sampling, use optimization!

Key point

- **KEY POINT 1** choose approximating distn to be **flexible**
- **KEY POINT 2** simple enough for efficient optimization

VI vs MCMC

MCMC :

- computationally intensive, but (asymptotically) exact samples
- suited to smaller dataset

VI :

- faster than MCMC (can use stochastic optimization), but do not guarantee exact samples
- suited to larger dataset
- when we want to quickly explore many models

Not only data size, but also **geometry of the posterior**

- multi-mode : VI > MCMC

Modern research in VI

- problem which involve massive data
- using improved optimization method
- easy to apply to a wide class of models
- increase the accuracy of VI (by stretching the boundaries of approx distn)

This paper...

- [Section 2] MVFI, CAVI
- [Section 3] Bayesian Mixture of Gaussians
- [Section 4-1&2] When joint density of z and x are exponential family
- [Section 4-3] SVI

3. Variational Inference

Goal of VI : approximate conditional density of latent variables, given observed variables (= $P(Z | X)$)

key : solve using **optimization**

(use family of densities over latent variables, parameterized by free **variational parameters**)

3-1. Problem of Approximate Inference

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

- evidence : $p(\mathbf{x}) = \int p(\mathbf{z}, \mathbf{x}) d\mathbf{z}$ (intractable)

Bayesian Mixture of Gaussians

- K mixture components
- mean params : $\mu = \{\mu_1, \dots, \mu_K\}$
 - drawn from $p(\mu_k) = \mathcal{N}(0, \sigma^2)$
- how to generate x_i ?
 - step 1) choose cluster assignment c_i
 - step 2) draw x_i from $\mathcal{N}(c_i^\top \mu, 1)$
- Full hierarchical model :
$$\begin{aligned} \mu_k &\sim \mathcal{N}(0, \sigma^2), & k &= 1, \dots, K, \\ c_i &\sim \text{Categorical}(1/K, \dots, 1/K), & i &= 1, \dots, n. \\ x_i | c_i, \mu &\sim \mathcal{N}(c_i^\top \mu, 1) & i &= 1, \dots, n \end{aligned}$$

- Joint pdf : (latent var : $\mathbf{z} = \{\mu, \mathbf{c}\}$)
$$p(\mu, \mathbf{c}, \mathbf{x}) = p(\mu) \prod_{i=1}^n p(c_i) p(x_i | c_i, \mu).$$
- Evidence :

$$p(\mathbf{x}) = \int p(\mu) \prod_{i=1}^n \sum_{c_i} p(c_i) p(x_i | c_i, \mu) d\mu$$

$$= \sum_c p(c) \int p(\mu) \prod_{i=1}^n p(x_i | c_i, \mu) d\mu$$

- time complexity of K -dim : $O(K^n)$

3-2. ELBO

Optimization problem ($q^*(\mathbf{z}) = \arg \min_{q(\mathbf{z}) \in \mathcal{Q}} \text{kL}(q(\mathbf{z}) || p(\mathbf{z} | \mathbf{x}))$)

Minimize KL Divergence :

$$\text{KL}(q(\mathbf{z}) || p(\mathbf{z} | \mathbf{x})) = \mathbb{E}[\log q(\mathbf{z})] - \mathbb{E}[\log p(\mathbf{z} | \mathbf{x})]$$

$$= \mathbb{E}[\log q(\mathbf{z})] - \mathbb{E}[\log p(\mathbf{z}, \mathbf{x})] + \log p(\mathbf{x})$$

Maximize ELBO:

$$\text{ELBO}(q) = \mathbb{E}[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}[\log q(\mathbf{z})]$$

Interpretation of ELBO :

$$\text{ELBO}(q) = \mathbb{E}[\log p(\mathbf{z})] + \mathbb{E}[\log p(\mathbf{x} | \mathbf{z})] - \mathbb{E}[\log q(\mathbf{z})]$$

$$= \mathbb{E}[\log p(\mathbf{x} | \mathbf{z})] - \text{kL}(q(\mathbf{z}) || p(\mathbf{z}))$$

- first term) fit well
- second term) regularize well

Relationship between ELBO & $\log p(x)$

- used for **model selection** criterion

EM vs VI

- EM assumes, expectation under $p(z | x)$ is computable
- VI does not estimate fixed-model parameters (classical params are treated as latent variables)

3-3. MFVI

Assumption : independency between latent variables

$$\rightarrow q(\mathbf{z}) = \prod_{j=1}^m q_j(z_j)$$

Each latent variable z_j is governed by its own variational factor, $q_j(z_j)$

(these variational factors are chosen to MAXIMIZE ELBO)

- ex) choose as Gaussian factor, or categorical factor

Researchers have also studied more complex families

- 1) Structured VI
- 2) Mixture of variational densities

→ both improve the fidelity of the approximation

(trade-off : difficult to solve variational optimization problem)

Bayesian Mixture of Gaussians (cont)

MFVI : $q(\mu, \mathbf{c}) = \prod_{k=1}^K q(\mu_k; m_k, s_k^2) \prod_{i=1}^n q(c_i; \varphi_i)$.

- $q(\mu_k; m_k, s_k^2)$: Gaussian distn
- $q(c_i; \varphi_i)$: its assignment probabilities are a K -vector φ_i

Summary : ELBO is defined by..

- model definition : $p(\mu, \mathbf{c}, \mathbf{x}) = p(\mu) \prod_{i=1}^n p(c_i) p(x_i | c_i, \mu)$
- MFVI : $q(\mu, \mathbf{c}) = \prod_{k=1}^K q(\mu_k; m_k, s_k^2) \prod_{i=1}^n q(c_i; \varphi_i)$

3-4. CAVI (Coordinate ascent MFVI)

CAVI : **iteratively** optimizes each factor of the MF variational density

optimal solution

- conditional : $q_j^*(z_j) \propto \exp\{\mathbb{E}_{-j}[\log p(z_j | \mathbf{z}_{-j}, \mathbf{x})]\}$.
 - joint : $q_j^*(z_j) \propto \exp\{\mathbb{E}_{-j}[\log p(z_j, \mathbf{z}_{-j}, \mathbf{x})]\}$.
- (expectation on RHS do not involve j^{th} variational factor → valid coordinate update)

Algorithm 1: Coordinate ascent variational inference (CAVI)

Input: A model $p(\mathbf{x}, \mathbf{z})$, a data set \mathbf{x}

Output: A variational density $q(\mathbf{z}) = \prod_{j=1}^m q_j(z_j)$

Initialize: Variational factors $q_j(z_j)$

while the ELBO has not converged **do**

for $j \in \{1, \dots, m\}$ **do**

 Set $q_j(z_j) \propto \exp\{\mathbb{E}_{-j}[\log p(z_j | \mathbf{z}_{-j}, \mathbf{x})]\}$

end

 Compute $\text{ELBO}(q) = \mathbb{E}[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}[\log q(\mathbf{z})]$

end

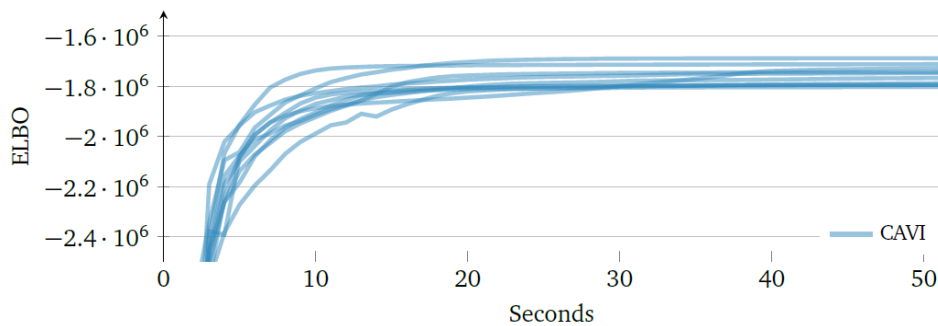
return $q(\mathbf{z})$

(can see that it is closely related to Gibbs sampling)

3-5. Practicalities

Initialization

- ELBO : (usually) non-convex objective function
- CAVI only guarantees local optimum (sensitive to initialization)



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- 10 random initialization, reaching different values!
(many local optima in ELBO)
- Not always bad!
 - ex) Mixture of Gaussian : many posterior modes
 - exploring latent clusters, predicting new observation

Assessing convergence

- computing the ELBO of full dataset may be undesirable
- proxy! average log predictive of a small held-out dataset

Numerical stability

- probabilities should be between 0~1
- use **log-sum-exp** trick
$$\log[\sum_i \exp(x_i)] = \alpha + \log[\sum_i \exp(x_i - \alpha)].$$

4. A complete example : Bayesian Mixture of Gaussians

notation

- K real valued mean params : $\mu = \mu_{1:K}$
- n latent class assignments : $\mathbf{c} = c_{1:n}$

ELBO for mixture of Gaussians

- variational parameters : $\mathbf{m}, \mathbf{s}^2, \varphi$

$$\begin{aligned}\text{ELBO}(\mathbf{m}, \mathbf{s}^2, \varphi) &= \sum_{k=1}^K \mathbb{E} [\log p(\mu_k); m_k, s_k^2] \\ &+ \sum_{i=1}^n (\mathbb{E} [\log p(c_i); \varphi_i] + \mathbb{E} [\log p(x_i | c_i, \mu); \varphi_i, \mathbf{m}, \mathbf{s}^2]) \\ &- \sum_{i=1}^n \mathbb{E} [\log q(c_i; \varphi_i)] - \sum_{k=1}^K \mathbb{E} [\log q(\mu_k; m_k, s_k^2)]\end{aligned}$$

CAVI updates each variational parameters in turn

4-1. (step 1)The variational density of the "mixture assignments"

(review) optimal solution : $q_j^*(z_j) \propto \exp\{\mathbb{E}_{-j} [\log p(z_j, \mathbf{z}_{-j}, \mathbf{x})]\}$

(1) derive variational update for c_i (cluster assignment)

- $q^*(c_i; \varphi_i) \propto \exp\{\log p(c_i) + \mathbb{E} [\log p(x_i | c_i, \mu); \mathbf{m}, \mathbf{s}^2]\}$.
 - 1st term) log prior of c_i : $\log p(c_i) = -\log K$
 - 2nd term) expected log of the c_i th Gaussian density

$$\blacksquare p(x_i | c_i, \mu) = \prod_{k=1}^K p(x_i | \mu_k)^{c_{ik}}$$

■ Thus,

$$\begin{aligned}\mathbb{E} [\log p(x_i | c_i, \mu)] &= \sum_k c_{ik} \mathbb{E} [\log p(x_i | \mu_k); m_k, s_k^2] \\ &= \sum_k c_{ik} \mathbb{E} \left[-(x_i - \mu_k)^2 / 2; m_k, s_k^2 \right] + \text{const.} \\ &= \sum_k c_{ik} (\mathbb{E} [\mu_k; m_k, s_k^2] x_i - \mathbb{E} [\mu_k^2; m_k, s_k^2] / 2) + \text{const.}\end{aligned}$$

- result : $\varphi_{ik} \propto \exp\{\mathbb{E} [\mu_k; m_k, s_k^2] x_i - \mathbb{E} [\mu_k^2; m_k, s_k^2] / 2\}$

4-2. (step 2)The variational density of the "mixture-component means"

(2) variational density $q(\mu_k; m_k, s_k^2)$ of k^{th} mixture components

$$q(\mu_k) \propto \exp\{\log p(\mu_k) + \sum_{i=1}^n \mathbb{E} [\log p(x_i | c_i, \mu); \varphi_i, \mathbf{m}_{-k}, \mathbf{s}_{-k}^2]\}.$$

Unnormallized log of $q(\mu_k)$:

$$\begin{aligned}
\log q(\mu_k) &= \log p(\mu_k) + \sum_i \mathbb{E} [\log p(x_i | c_i, \mu); \varphi_i, \mathbf{m}_{-k}, \mathbf{s}_{-k}^2] + \text{const.} \\
&= \log p(\mu_k) + \sum_i \mathbb{E} [c_{ik} \log p(x_i | \mu_k); \varphi_i] + \text{const.} \\
&= -\mu_k^2/2\sigma^2 + \sum_i \mathbb{E} [c_{ik}; \varphi_i] \log p(x_i | \mu_k) + \text{const.} \\
&= -\mu_k^2/2\sigma^2 + \sum_i \varphi_{ik} \left(-(x_i - \mu_k)^2/2 \right) + \text{const.} \\
&= -\mu_k^2/2\sigma^2 + \sum_i \varphi_{ik} x_i \mu_k - \varphi_{ik} \mu_k^2/2 + \text{const.} \\
&= \left(\sum_i \varphi_{ik} x_i \right) \mu_k - \left(1/2\sigma^2 + \sum_i \varphi_{ik}/2 \right) \mu_k^2 + \text{const.}
\end{aligned}$$

where $\varphi_{ik} = \mathbb{E} [c_{ik}; \varphi_i]$.

Thus, $m_k = \frac{\sum_i \varphi_{ik} x_i}{1/\sigma^2 + \sum_i \varphi_{ik}}, \quad s_k^2 = \frac{1}{1/\sigma^2 + \sum_i \varphi_{ik}}$

4-3. CAVI for the mixture of Gaussians

Algorithm 2: CAVI for a Gaussian mixture model

Input: Data $x_{1:n}$, number of components K , prior variance of component means σ^2

Output: Variational densities $q(\mu_k; m_k, s_k^2)$ (Gaussian) and $q(c_i; \varphi_i)$ (K -categorical)

Initialize: Variational parameters $\mathbf{m} = m_{1:K}$, $\mathbf{s}^2 = s_{1:K}^2$, and $\varphi = \varphi_{1:n}$

while the ELBO has not converged **do**

```

for  $i \in \{1, \dots, n\}$  do
    | Set  $\varphi_{ik} \propto \exp\{\mathbb{E}[\mu_k; m_k, s_k^2] x_i - \mathbb{E}[\mu_k^2; m_k, s_k^2]/2\}$ 
end
for  $k \in \{1, \dots, K\}$  do
    |
    |   Set  $m_k \leftarrow \frac{\sum_i \varphi_{ik} x_i}{1/\sigma^2 + \sum_i \varphi_{ik}}$ 
    |   Set  $s_k^2 \leftarrow \frac{1}{1/\sigma^2 + \sum_i \varphi_{ik}}$ 
    |
end
    Compute ELBO( $\mathbf{m}, \mathbf{s}^2, \varphi$ )

```

end

return $q(\mathbf{m}, \mathbf{s}^2, \varphi)$

Approximate predictive : (mixture of Gaussians)

$$p(x_{\text{new}} | x_{1:n}) \approx \frac{1}{K} \sum_{k=1}^K p(x_{\text{new}} | m_k)$$

5. VI with exponential families

(Until now....)

- **MFVI**
- **CAVI** (coordinate ascent algorithm for optimizing ELBO)

- demonstration using **simple mixture of Gaussians**
(available in closed-form)

Now, will work with **exponential family**

- working with this simplifies VI
- easier to derive CAVI
- section 5-1) general case
section 5-2) conditionally conjugate models
section 5-3) SVI

5-1. Complete conditionals in the exponential family

suppose **complete conditional** is "exponential family" :

$$p(z_j | \mathbf{z}_{-j}, \mathbf{x}) = h(z_j) \exp\left\{\eta_j(\mathbf{z}_{-j}, \mathbf{x})^\top z_j - a(\eta_j(\mathbf{z}_{-j}, \mathbf{x}))\right\}$$

CAVI with MFVI

- coordinate update of $q_j^*(z_j) \propto \exp\{\mathbb{E}_{-j}[\log p(z_j | \mathbf{z}_{-j}, \mathbf{x})]\} =$
 $q(z_j) \propto \exp\{\mathbb{E}[\log p(z_j | \mathbf{z}_{-j}, \mathbf{x})]\}$
 $= \exp\left\{\mathbb{E}\left[\log h(z_j) \exp\left\{\eta_j(\mathbf{z}_{-j}, \mathbf{x})^\top z_j - a(\eta_j(\mathbf{z}_{-j}, \mathbf{x}))\right\}\right]\right\}$
 $= \exp\left\{\log h(z_j) + \mathbb{E}[\eta_j(\mathbf{z}_{-j}, \mathbf{x})]^\top z_j - \mathbb{E}[a(\eta_j(\mathbf{z}_{-j}, \mathbf{x}))]\right\}$
 $\propto h(z_j) \exp\left\{\mathbb{E}[\eta_j(\mathbf{z}_{-j}, \mathbf{x})]^\top z_j\right\}$
- set $v_j = \mathbb{E}[\eta_j(\mathbf{z}_{-j}, \mathbf{x})]$

5-2. Conditional conjugacy and Bayesian models

Special case of exponential family : "conditional conjugate models" with local & global variables

Conditionally conjugate models

- β : global latent variables
- \mathbf{z} : local latent variables
- joint pdf : $p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^n p(z_i, x_i | \beta)$

Assumption 1) joint density of each (x_i, z_i) pair, conditional on β = exponential family

$$p(z_i, x_i | \beta) = h(z_i, x_i) \exp\{\beta^\top t(z_i, x_i) - a(\beta)\} \dots \dots \dots (a)$$

Assumption 2) prior (on global variables) to be conjugate prior

$$p(\beta) = h(\beta) \exp\{\alpha^\top [\beta, -a(\beta)] - a(\alpha)\} \dots\dots\dots (b)$$

- natural (hyper) parameter $\alpha = [\alpha_1, \alpha_2]^\top$

(a) and (b) : conjugate $\rightarrow \hat{\alpha} = [\alpha_1 + \sum_{i=1}^n t(z_i, x_i), \alpha_2 + n]^\top$

Complete conditional of local variable z_i :

- (given β and x_i) z_i is conditionally independent!
 $\rightarrow p(z_i | x_i, \beta, \mathbf{z}_{-i}, \mathbf{x}_{-i}) = p(z_i | x_i, \beta)$
- assumption) exponential family
 $\rightarrow p(z_i | x_i, \beta) = h(z_i) \exp\{\eta(\beta, x_i)^\top z_i - a(\eta(\beta, x_i))\}$

VI in conditionally conjugate models

describe CAVI for general class of models

notation

- λ : **global** variational parameter
 $q(\beta | \lambda)$: variational posterior approximation on β
- ϕ : **local** variational parameter
 $q(z_i | \phi)$: variational posterior on each local variable z_i

Local variational update : $\varphi_i = \mathbb{E}_\lambda [\eta(\beta, x_i)]$ by

- (1) $v_j = \mathbb{E} [\eta_j(\mathbf{z}_{-j}, \mathbf{x})]$
- (2) $p(z_i | x_i, \beta, \mathbf{z}_{-i}, \mathbf{x}_{-i}) = p(z_i | x_i, \beta)$

Global variational update : $\lambda = [\alpha_1 + \sum_{i=1}^n \mathbb{E}_{\varphi_i} [t(z_i, x_i)], \alpha_2 + n]^\top$

- expectation of $\hat{\alpha} = [\alpha_1 + \sum_{i=1}^n t(z_i, x_i), \alpha_2 + n]^\top$

CAVI optimizes the ELBO by iterating "local updates" and "global updates"

To assess convergence, compute ELBO at each iteration!

ELBO :

- $\text{ELBO}(q) = \mathbb{E}[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}[\log q(\mathbf{z})]$
 $p(\beta, \mathbf{z}, \mathbf{x}) = p(\beta) \prod_{i=1}^n p(z_i, x_i | \beta)$
- Therefore, $\text{ELBO} = (\alpha_1 + \sum_{i=1}^n \mathbb{E}_{\varphi_i} [t(z_i, x_i)])^\top \mathbb{E}_\lambda [\beta] - (\alpha_2 + n) \mathbb{E}_\lambda [a(\beta)] - \mathbb{E}[\log q(\beta, \mathbf{z})]$
 - $\mathbb{E}[\log q(\beta, \mathbf{z})] = \lambda^\top \mathbb{E}_\lambda [t(\beta)] - a(\lambda) + \sum_{i=1}^n \varphi_i^\top \mathbb{E}_{\varphi_i} [z_i] - a(\varphi_i)$

5-3. SVI (Stochastic Variational Inference)

Modern problems : require analyzing massive data

but, most do not easily scale (ex. CAVI)

CAVI, not scalable!

- requires iteration through entire data at each iteration
- alternative : **gradient-based optimization**
(= Key to SVI)

SVI focuses on optimizing the global variational params λ of conditionally conjugate model

- step 1) subsample data
- step 2) use current global param to compute **optimal local params** for the subsampled data
- step 3) adjust the current **global params**

Natural gradient of ELBO

SVI focuses on optimizing the global variational params λ

Euclidan gradient of ELBO :

- $\nabla_{\lambda} \text{ELBO} = a''(\lambda) (\mathbb{E}_{\varphi}[\hat{\alpha}] - \lambda)$ (Hoffman et al. 2013)

Natural gradient : (premultiply by inverse Fisher info)

- $g(\lambda) = \mathbb{E}_{\varphi}[\hat{\alpha}] - \lambda$

Update param, using **natural gradient** in gradient-based optimization method

- at each iteration, update $\lambda_t = \lambda_{t-1} + \epsilon_t g(\lambda_{t-1})$
(= $\lambda_t = (1 - \epsilon_t) \lambda_{t-1} + \epsilon_t \mathbb{E}_{\varphi}[\hat{\alpha}]$)

Stochastic Optimization of the ELBO

goal : construct a cheaply computed, noisy, unbiased natural gradient

- $g(\lambda) = \mathbb{E}_{\varphi}[\hat{\alpha}] - \lambda$
- $\hat{\alpha} = [\alpha_1 + \sum_{i=1}^n t(z_i, x_i), \alpha_2 + n]^{\top}$

$$\rightarrow g(\lambda) = \alpha + \left[\sum_{i=1}^n \mathbb{E}_{\varphi_i^*} [t(z_i, x_i)], n \right]^{\top} - \lambda$$

(φ_i^* : optimized local variational param)

Construct noisy natural gradient, by **sampling an index from the data** & rescaling

- $t \sim \text{Unif}(1, \dots, n)$

$$\hat{g}(\lambda) = \alpha + n [\mathbb{E}_{\varphi_t^*} [t(z_t, x_t)], 1]^\top - \lambda$$

- $\hat{g}(\lambda)$ is unbiased ($\mathbb{E}_t[\hat{g}(\lambda)] = g(\lambda)$) & cheap to compute
(not only sample 1 data, but can also use mini-batch)

Step-size sequence

- should follow conditions of Robbins and Monro,

$$\sum_t \epsilon_t = \infty; \sum_t \epsilon_t^2 < \infty$$

Algorithm 3: svi for conditionally conjugate models

Input: Model $p(\mathbf{x}, \mathbf{z})$, data \mathbf{x} , and step size sequence ϵ_t

Output: Global variational densities $q_\lambda(\beta)$

Initialize: Variational parameters λ_0

while *TRUE* **do**

 Choose a data point uniformly at random, $t \sim \text{Unif}(1, \dots, n)$

 Optimize its local variational parameters $\varphi_t^* = \mathbb{E}_\lambda [\eta(\beta, x_t)]$

 Compute the coordinate update as though x_t was repeated n times,

$$\hat{\lambda} = \alpha + n \mathbb{E}_{\varphi_t^*} [f(z_t, x_t)]$$

 Update the global variational parameter, $\lambda_t = (1 - \epsilon_t)\lambda_t + \epsilon_t \hat{\lambda}_t$

end

return λ

6. Discussion

Summary

- MFVI
- CAVI
- Bayesian Mixture of Gaussians
- special case of exponential families & conditional conjugacy
- SVI