

Solving Inverse Problems by VAE-like Approaches

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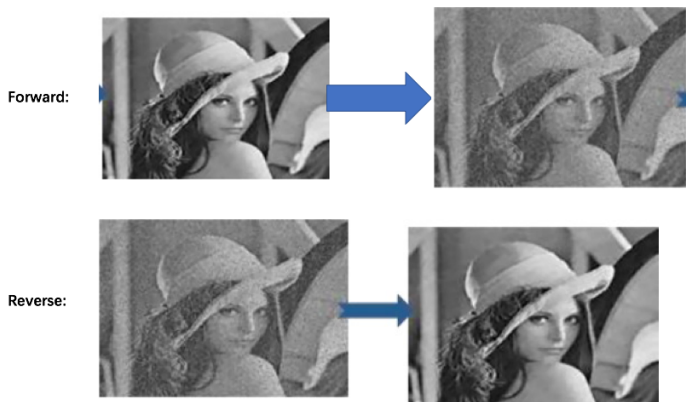
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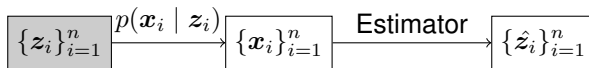
Motivation

- Inverse problems refer to the *reverse process* of a forward problem.
- Example:



Inverse Problem in Statistics

- $z \sim g(z; \Lambda)$ with the unknown parameter Λ
- x is generated through a known likelihood model $p(x | z)$:
- Given n observed data points $\{x_i\}_{i=1}^n$, recover $\{z_i\}_{i=1}^n$.



- Example: $z \sim g(z; \Lambda)$, and $x | z \sim \mathcal{N}(z, \sigma^2 I)$.

If given observations $\{x_i\}_{i=1}^n$, then what is $\{z_i\}_{i=1}^n$?

① Naive idea: $z_i \approx x_i$

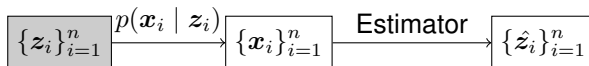
② Non-trivial idea:

★ order $\{x_i\}_{i=1}^n$ from smallest to largest, say $\{x_{(i)}\}_{i=1}^n$

★ $\hat{z}_i = x_{(i)}$

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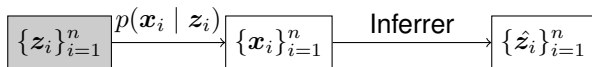
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Empirical Bayes approach

- Given n observed data points $\{\mathbf{x}_i\}_{i=1}^n$, aim to recover $\{\mathbf{z}_i\}_{i=1}^n$:

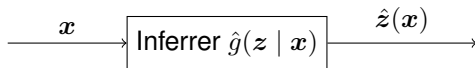


- Empirical Bayes:**

Estimation:



Inference:



G-modelling for Empirical Bayes

Estimation:



The estimation problem relies on maximizing the marginal likelihood:

$$\hat{\Lambda} = \arg \max_{\Lambda} \sum_{i=1}^n \log p(\mathbf{x}_i) \triangleq \max \sum_{i=1}^n \log \int g(z_i; \Lambda) p(\mathbf{x}_i | z_i) dz_i \quad (1)$$

Intractable for complicated prior distribution or high dimension latent space!

G-modelling for Empirical Bayes

Estimation:

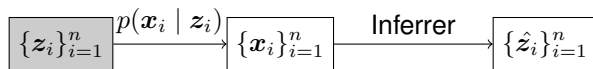


The estimation problem relies on maximizing the marginal likelihood:

$$\hat{\Lambda} = \arg \max_{\Lambda} \sum_{i=1}^n \log p(\mathbf{x}_i) \triangleq \max_{\Lambda} \sum_{i=1}^n \log \int g(\mathbf{z}_i; \Lambda) p(\mathbf{x}_i | \mathbf{z}_i) d\mathbf{z}_i \quad (1)$$

Intractable for complicated prior distribution or high dimension latent space!

Variational Inference Approach



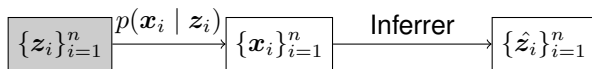
- Jointly perform the estimation and inference task:

$$\log p(\mathbf{x}; \mathbf{\Lambda}) \geq \mathbb{E}_{q_\phi(\mathbf{z})} [\log p(\mathbf{z}; \mathbf{\Lambda}) + \log p(\mathbf{x} | \mathbf{z}) - \log q_\phi(\mathbf{z})] \triangleq \text{ELBO}(\mathbf{x}; \mathbf{\Lambda}, \phi)$$

where $q_\phi(\mathbf{z})$ is the approximation of the true posterior $p(\mathbf{z} | \mathbf{x}; \mathbf{\Lambda})$.

- The optimization for ELBO relies on *mean-field approximation* technique:
 - 1 Large suboptimality Gap, and therefore unreliable estimator and inferer
 - 2 Non-convexity Landscape with local optimal points
 - 3 No reparametrization trick! Complicated simplification on ELBO

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Vanilla VAE-like approach

- Maximize the ELBO function via stochastic optimization techniques:

$$(\hat{\Lambda}, \hat{\phi}) = \arg \max_{\Lambda, \phi} \sum_{i=1}^n \mathbb{E}_{q_{\phi}(\mathbf{z}_i | \mathbf{x}_i)} \left[\log g(\mathbf{z}_i; \Lambda) + \log p(\mathbf{x}_i | \mathbf{z}_i) - \log q_{\phi}(\mathbf{z}_i | \mathbf{x}_i) \right]$$

where:

- $g(\mathbf{z}_i; \Lambda)$ and $p(\mathbf{x}_i | \mathbf{z}_i)$ is known
- $q_{\phi}(\mathbf{z}_i | \mathbf{x}_i)$ is the approximation of the true posterior $p(\mathbf{z} | \mathbf{x}; \Lambda)$:

$$(\boldsymbol{\mu}_{1:n}, \log \boldsymbol{\sigma}_{1:n}) = \text{Encoder-Neural-Net}_{\phi}(\mathbf{x}_{1:n});$$

$$q_{\phi}(\mathbf{z} | \mathbf{x}) = \prod_{i=1}^n q_{\phi}(\mathbf{z}_i | \mathbf{x}_i) = \prod_{i=1}^n \mathcal{N}(\boldsymbol{\mu}_i, \text{diag}(\boldsymbol{\sigma}_i^2));$$

$$q_{\phi}(\mathbf{z} | \mathbf{x}) \approx p(\mathbf{z} | \mathbf{x}; \Lambda).$$

- Optimize for ϕ : reparametrization trick $\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \circ \boldsymbol{\epsilon}$ with $\boldsymbol{\epsilon} \sim \mathcal{N}(0, 1)$
- Optimize for Λ : parametric optimization techniques

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Vanilla VAE-like approach

Algorithm 1 Algorithm for Vanilla VAE-like approach. All experiments in the paper used the default values $\alpha = 0.000001$, $B = 128$, $n_{\text{critic}} = 30$

Input: $\{x_i\}_{i=1}^n$, observations; $p(x \mid z)$, generative model; η , learning rate; n_{critic} , the number of iterations of the ϕ update per Λ estimation.

Output: $\hat{\Lambda}, \hat{\phi}$: learnt parameters

```

1:  $\hat{\Lambda}, \hat{\phi} \leftarrow$  initialize parameters
2: while Adam not converged do
3:   for  $t = 0, \dots, n_{\text{critic}}$  do
4:     Sample  $\{x_{(i)}\}_{i=1}^B$ , a batch from the real data
5:     Sample random noise  $\epsilon \sim p(\epsilon)$ 
6:     Generate  $\{z_{(i)}\}_{i=1}^B$  by the reparameterisation trick  $z = \mu + \sigma \circ \epsilon$ 
7:     Compute the objective function  $\tilde{L}_{\Lambda, \phi}(\{x_{(i)}\}_{i=1}^B, \{z_{(i)}\}_{i=1}^B)$  and its gradients  $\nabla_{\phi} \tilde{L}_{\Lambda, \phi}$ :

```

$$\tilde{L}_{\Lambda, \phi}(\{x_{(i)}\}_{i=1}^B, \{z_{(i)}\}_{i=1}^B) \triangleq \sum_{i=1}^B -\log(z_{(i)}; \Lambda) - \log p(x_{(i)} \mid z_{(i)}) - \sum_j \log |\sigma_{(i), j}| \quad (4a)$$

```

8:     Update  $\hat{\phi}$  using Adam optimizer
9:   end for
10:  Sample  $\{x_{(i)}\}_{i=1}^B$ , a batch from the real data and random noise  $\epsilon \sim p(\epsilon)$ 
11:  Generate  $\{z_{(i)}\}_{i=1}^B$  by the reparameterisation trick
12:  Update  $\Lambda$  by solving the maximization problem

```

$$\hat{\Lambda} = \arg \max_{\Lambda} \sum_{i=1}^B \log(z_{(i)}; \Lambda) \quad (4b)$$

```

13: end while

```


VAE-like approach with Inverse Autoregressive Flow

- Vanilla VAE-like approach suffices from the inexact approximation posterior.
- Circumvent it by the Inverse Autoregressive Flow trick:

$$\begin{aligned}\epsilon_0 &\sim \mathcal{N}(0, \mathbf{I}), \\ (\mu_0, \log(\sigma_0), \mathbf{h}) &= \text{Encoder-Neural-Net}(\mathbf{x}; \psi) \\ \mathbf{z}_0 &= \mu_0 + \sigma_0 \circ \epsilon_0\end{aligned}$$

Then apply the following transformations for $t = 1, \dots, T$:

$$\begin{aligned}(\mathbf{m}_t, \mathbf{s}_t) &= \text{Auto-regressive-Neural-Net}_t(\epsilon_{t-1}, \mathbf{h}; \psi) \\ \sigma_t &= \text{sigmoid}(\mathbf{s}_t) \\ \epsilon_t &= \sigma_t \circ \epsilon_{t-1} + (1 - \sigma_t) \circ \mathbf{m}_t\end{aligned}$$

and finally $\mathbf{z} \triangleq \epsilon_t$.

- 1 increases flexibility of approximation posteriors
- 2 scales well to a high-dimensional latent space
- 3 easy-to-implement by using the open source library

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VAE-like approach with Inverse Autoregressive Flow

Two things to be modified based on Vanilla VAE approach:

$$(\hat{\Lambda}, \hat{\phi}) = \arg \max_{\Lambda, \phi} \sum_{i=1}^n \mathbb{E}_{q_{\phi}(z_i | x_i)} \left[\log g(z_i; \Lambda) + \log p(x_i | z_i) - \log q_{\phi}(z_i | x_i) \right]$$

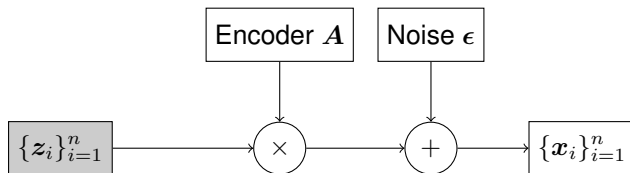
- 1 The generation of z via $q_{\phi}(z_i | x_i)$ is from the Inverse Autoregressive Flow process;
- 2 Substitute the evaluation for the term $\log q_{\phi}(z_i | x_i)$:

$$\log q_{\phi}(z \triangleq \epsilon_T | x) = - \sum_{i=1}^n \left(\frac{1}{2} \epsilon_i^2 + \frac{1}{2} \log(2\pi) + \sum_{t=0}^T \sigma_{t,i} \right)$$

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Problem Setting



(Latent Space) $z_i \sim \mathcal{N}(\mathbf{0}, \Lambda^{-1}), \quad \Lambda \text{ sparse},$
 (Observation Space) $x_i \mid z_i \sim \mathcal{N}(\mathbf{A}_{\text{obs}} z_i, \sigma_{\text{obs}}^2 \mathbf{I})$

Vanilla VAE-like Approach

- 1 Estimation for $\phi := (\boldsymbol{\mu}, \boldsymbol{\sigma}^2)$: generate $\mathbf{z}_{(i)}$'s and then minimize

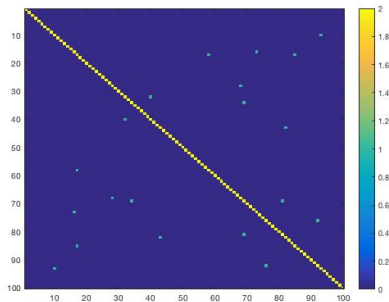
$$\frac{1}{2} \text{Trace} \left(\boldsymbol{\Lambda} \cdot \sum_{i=1}^B (\mathbf{z}_{(i)}) (\mathbf{z}_{(i)})^T \right) + \frac{1}{2\sigma_{\text{obs}}^2} \sum_{i=1}^B \|\mathbf{x}_{(i)} - \mathbf{A}_{\text{obs}} \mathbf{z}_{(i)}\|^2 - \sum_{i=1, j}^B \log |\sigma_{(i),j}|$$

- 2 Estimation for $\boldsymbol{\Lambda}$: generate $\mathbf{z}_{(i)}$'s and then solve the graphical lasso subproblem:

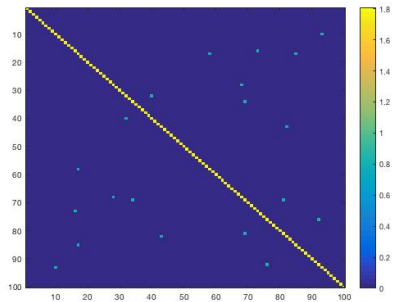
$$\arg \max_{\boldsymbol{\Lambda}} -\lambda \cdot \|\boldsymbol{\Lambda}\|_{\ell_1, \text{off}} + \frac{B}{2} \log |\boldsymbol{\Lambda}| - \frac{B}{2} \text{Trace} \left[\boldsymbol{\Lambda} \cdot \frac{1}{B} \sum_{i=1}^B (\mathbf{z}_{(i)}) (\mathbf{z}_{(i)})^T \right]$$

Disadvantage: graphical lasso problem is computationally expansive!

Simulation Results



(a) Underlying Precision matrix Λ_{true}



(b) Estimated Precision matrix $\hat{\Lambda}$

Simulation Results

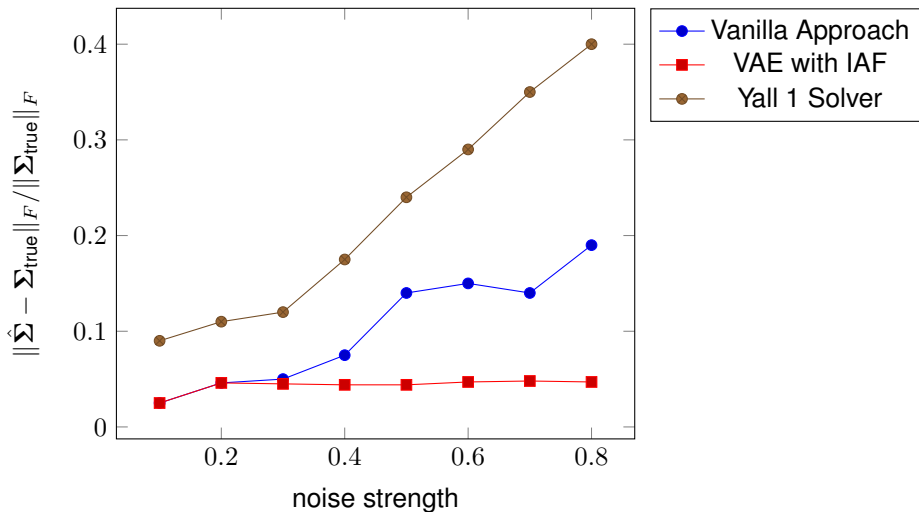
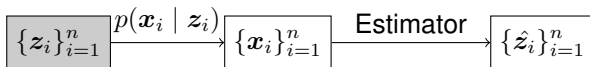


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Future Work

- Consider the signal reconstruction task from Gaussian Mixture Model:



where

$$\mathbf{z} \sim \sum_{i=1}^K \pi_i \cdot \mathcal{N}(\mathbf{0}, \mathbf{\Lambda}_{(K)}^{-1})$$

- Consider the more general likelihood function $p(\mathbf{x} | \mathbf{z})$. For instance, the inverse problem can be used for solving stochastic differential equation:

$$\mathbf{x} = \mathcal{G}(\mathbf{z}, \epsilon),$$

where $\mathcal{G}(\cdot)$ is the generative model, ϵ is the random noise, and \mathbf{x} are observed data points.

Concluding Remarks

- The inverse problem is an old problem studied in history, and we use VAE-like approach to efficiently solve it;
- Such approach is applicable to general prior distribution patterns and likelihood models
- The suboptimality gap for this approach is an open problem.