Solving Inverse Problems by VAE-like Approaches

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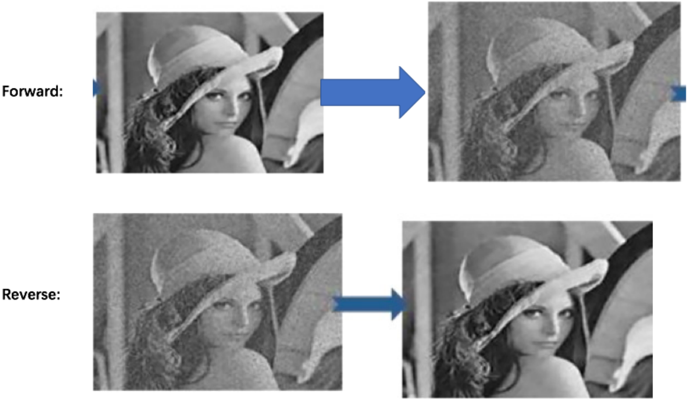
Motivation

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



Inverse Problem in Statistics

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

$$\boxed{\{\boldsymbol{z}_i\}_{i=1}^n} \xrightarrow{p(\boldsymbol{x}_i \mid \boldsymbol{z}_i)} \boxed{\{\boldsymbol{x}_i\}_{i=1}^n} \xrightarrow{\text{Estimator}} \boxed{\{\hat{\boldsymbol{z}}_i\}_{i=1}^n}$$

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

  If given observations $\{\boldsymbol{x}_i\}_{i=1}^n$, then what is $\{\boldsymbol{z}_i\}_{i=1}^n$?

  1. Naive idea: $\boldsymbol{z}_i \approx \boldsymbol{x}_i$
  2. Non-trivial idea:
     - order $\{\boldsymbol{x}_i\}_{i=1}^n$ from smallest to largest, say $\{\boldsymbol{x}_{(i)}\}_{i=1}^n$
     - $\hat{\boldsymbol{z}}_i = \boldsymbol{x}_{(i)}$

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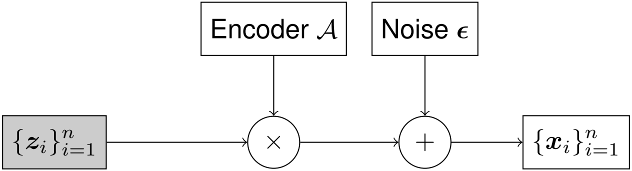
Hard Inverse Problems



- The likelihood model $\boldsymbol{x} \mid \boldsymbol{z}$ can be represented as $\boldsymbol{x} = \mathcal{G}(\boldsymbol{z}) + \boldsymbol{\epsilon}$. Given a specified encoder, how to train a decoder with low complexity?
- Stochastic differential equations can be solved via the inverse problem:

$$\boldsymbol{x}[t] = \mathcal{G}(\boldsymbol{x}[t+1], \boldsymbol{\epsilon}),$$

  where $\boldsymbol{x}[t]$ is observed, and we want to derive $\boldsymbol{x}[t+1]$.
- We present a simulation for a linear inverse problem.

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Empirical Bayes approach

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

$$\boxed{\{\boldsymbol{z}_i\}_{i=1}^n} \xrightarrow{p(\boldsymbol{x}_i \mid \boldsymbol{z}_i)} \boxed{\{\boldsymbol{x}_i\}_{i=1}^n} \xrightarrow{\text{Inferrer}} \boxed{\{\hat{\boldsymbol{z}}_i\}_{i=1}^n}$$

- **Empirical Bayes**:

Estimation:

$$\boxed{\{\boldsymbol{z}_i\}_{i=1}^n} \xrightarrow{p(\boldsymbol{x}_i \mid \boldsymbol{z}_i)} \boxed{\{\boldsymbol{x}_i\}_{i=1}^n} \longrightarrow \boxed{\text{Estimator}} \xrightarrow{\hat{g}(\boldsymbol{z}) := g(\boldsymbol{z}; \hat{\boldsymbol{\Lambda}})}$$

Inference:

$$\xrightarrow{\boldsymbol{x}} \boxed{\text{Inferrer } \hat{g}(\boldsymbol{z} \mid \boldsymbol{x})} \xrightarrow{\hat{z}(\boldsymbol{x})}$$

G-modelling for Empirical Bayes

Estimation:

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The estimation problem relies on maximizing the marginal likelihood:

$$\hat{\boldsymbol{\Lambda}} = \arg\max_{\boldsymbol{\Lambda}} \sum_{i=1}^{n} \log p(\boldsymbol{x}_i) \triangleq \max \sum_{i=1}^{n} \log \int g(\boldsymbol{z}_i; \boldsymbol{\Lambda}) p(\boldsymbol{x}_i \mid \boldsymbol{z}_i) \, \mathrm{d}\boldsymbol{z}_i \tag{1}$$

Intractable for complicated prior distribution or high dimension latent space!

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Variational Inference Approach

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- Jointly perform the estimation and inference task:

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

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

- The optimization for ELBO relies on *mean-field approximation* technique:
  1. Large suboptimality Gap, and therefore unreliable estimator and inferrer
  2. Non-convexity Landscape with local optimal points
  3. Limited Choice of posterior approximation.

Variational Inference Approach

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Vanilla VAE-like approach

- Maximize the ELBO function via stochastic optimization techniques:

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

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

$$\begin{aligned}(\boldsymbol{\mu}_{1:n}, \log \boldsymbol{\sigma}_{1:n}) &= \text{Encoder-Neural-Net}_\phi(\boldsymbol{x}_{1:n});\\ q_\phi(\boldsymbol{z} \mid \boldsymbol{x}) &= \prod_{i=1}^{n} q_\phi(\boldsymbol{z}_i \mid \boldsymbol{x}_i) = \prod_{i=1}^{n} \mathcal{N}(\boldsymbol{\mu}_i, \text{diag}(\boldsymbol{\sigma}_i^2));\\ q_\phi(\boldsymbol{z} \mid \boldsymbol{x}) &\approx p(\boldsymbol{z} \mid \boldsymbol{x}; \Lambda).\end{aligned}$$

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

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$$q_\phi(\boldsymbol{z} \mid \boldsymbol{x}) \approx p(\boldsymbol{z} \mid \boldsymbol{x}; \Lambda).$$

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

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

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

```
Λ̂, φ̂ ← initialize parameters
while Adam not converged do
    for t = 0, ..., n_critic do
        Sample {x_(i)}_{i=1}^B, a batch from the real data
        Sample random noise ε ~ p(ε)
        Generate {z_(i)}_{i=1}^B by the reparameriation trick z = μ + σ ∘ ε
        Compute the objective function L̃_{Λ,φ}({x_(i)}_{i=1}^B, {z_(i)}_{i=1}^B) and its gradients ∇_φ L̃_{Λ,φ}:
```

$$\tilde{L}_{\boldsymbol{\Lambda},\boldsymbol{\phi}}(\{x_{(i)}\}_{i=1}^B, \{z_{(i)}\}_{i=1}^B) \triangleq \sum_{i=1}^{B} -\log(\boldsymbol{z}_{(i)}; \boldsymbol{\Lambda}) - \log p(\boldsymbol{x}_{(i)} \mid \boldsymbol{z}_{(i)}) - \sum_{j} \log |\boldsymbol{\sigma}_{(i),j}| \tag{4a}$$

```
        Update φ̂ using Adam optimizer
    end for
    Sample {x_(i)}_{i=1}^B, a batch from the real data and random noise ε ~ p(ε)
    Generate {z_(i)}_{i=1}^B by the reparameriation trick
    Update Λ by solving the maximization problem
```

$$\hat{\boldsymbol{\Lambda}} = \arg\max_{\boldsymbol{\Lambda}} \sum_{i=1}^{B} \log(\boldsymbol{z}_{(i)}; \boldsymbol{\Lambda}) \tag{4b}$$

```
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:

$$\begin{aligned}
\boldsymbol{\epsilon}_0 &\sim \mathcal{N}(0, \boldsymbol{I}), \\
(\boldsymbol{\mu}_0, \log(\boldsymbol{\sigma}_0), \boldsymbol{h}) &= \text{Encoder-Neural-Net}(\boldsymbol{x}; \psi) \\
\boldsymbol{z}_0 &= \boldsymbol{\mu}_0 + \boldsymbol{\sigma}_0 \circ \boldsymbol{\epsilon}_0
\end{aligned}$$

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

$$\begin{aligned}
(\boldsymbol{m}_t, \boldsymbol{s}_t) &= \text{Auto-regressive-Neural-Net}_t(\boldsymbol{\epsilon}_{t-1}, \boldsymbol{h}; \psi) \\
\boldsymbol{\sigma}_t &= \text{sigmoid}(\boldsymbol{s}_t) \\
\boldsymbol{\epsilon}_t &= \boldsymbol{\sigma}_t \circ \boldsymbol{\epsilon}_{t-1} + (1 - \boldsymbol{\sigma}_t) \circ \boldsymbol{m}_t
\end{aligned}$$

and finally $\boldsymbol{z} \triangleq \boldsymbol{\epsilon}_t$.

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:

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

1. The generation of $\boldsymbol{z}$ via $q_\phi(\boldsymbol{z}_i \mid \boldsymbol{x}_i)$ is from the Inverse Autoregressive Flow process;
2. Substitute the evaluation for the term $\log q_\phi(\boldsymbol{z}_i \mid \boldsymbol{x}_i)$:

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

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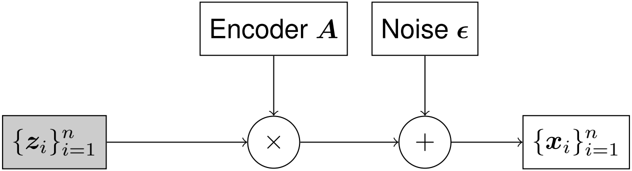
Problem Setting



$$\begin{aligned} &\text{(Latent Space)} && \boldsymbol{z}_i \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Lambda}^{-1}), \quad \boldsymbol{\Lambda} \text{ sparse}, \\ &\text{(Observation Space)} && \boldsymbol{x}_i \mid \boldsymbol{z}_i \sim \mathcal{N}(\boldsymbol{A}_{\text{obs}}\boldsymbol{z}_i, \sigma^2_{\text{obs}}\boldsymbol{I}) \end{aligned}$$

Vanilla VAE-like Approach

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

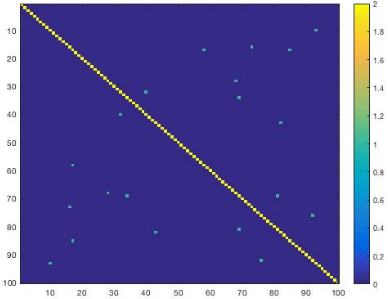
$$\frac{1}{2}\,\text{Trace}\left(\boldsymbol{\Lambda}\cdot\sum_{i=1}^{B}(\boldsymbol{z}_{(i)})(\boldsymbol{z}_{(i)})^{\mathrm{T}}\right)+\frac{1}{2\sigma_{\text{obs}}^2}\sum_{i=1}^{B}\|\boldsymbol{x}_{(i)}-\boldsymbol{A}_{\text{obs}}\boldsymbol{z}_{(i)}\|^2-\sum_{i=1,j}^{B}\log|\sigma_{(i),j}|$$

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

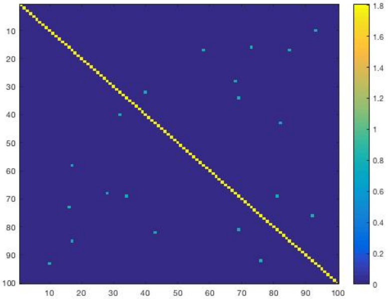
$$\arg\max_{\boldsymbol{\Lambda}}\quad -\lambda\cdot\|\boldsymbol{\Lambda}\|_{\ell_1,\text{off}}+\frac{B}{2}\log|\boldsymbol{\Lambda}|-\frac{B}{2}\,\text{Trace}\left[\boldsymbol{\Lambda}\cdot\frac{1}{B}\sum_{i=1}^{B}(\boldsymbol{z}_{(i)})(\boldsymbol{z}_{(i)})^{\mathrm{T}}\right]$$

Disadvantage: graphical lasso problem is computationally expansive!

Simulation Results



(a) Underlying Precision matrix $\boldsymbol{\Lambda}_{\text{true}}$



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

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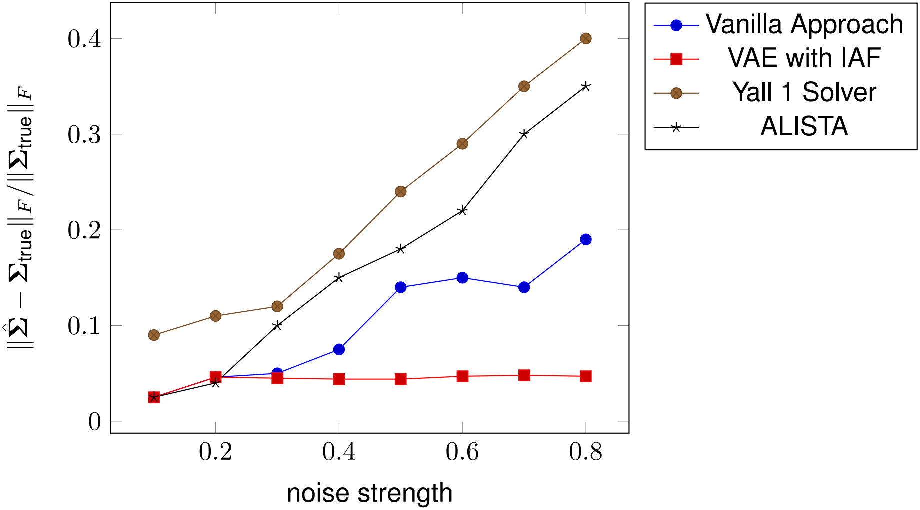

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Future Work

- Consider the inverse problem where the prior is a Gaussian Mixture Model:

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  where

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

- stochastic differential equation solver;
- real data testing

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 and the generalization bound for this approach is an open problem.