# Solving Inverse Problems by Amortized Variational Inference

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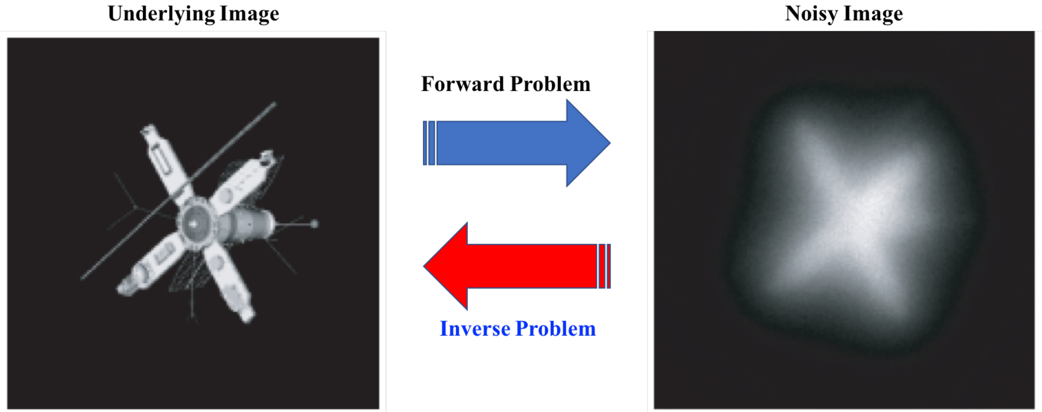
# Motivation

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



# Statistical Framework for Inverse Problems

- $\boldsymbol{z} \sim g(\boldsymbol{z}; \boldsymbol{\Lambda})$ 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: $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{z}; \boldsymbol{0}, A\boldsymbol{I})$, 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: $\boldsymbol{z}_i^{(\text{MLE})} = \boldsymbol{x}_i$
  2. Non-trivial idea:

$$\boldsymbol{z}_i^{(\text{JS})} = \left(1 - \frac{(n-2)\sigma^2}{\|\boldsymbol{x}_i\|^2}\right)\boldsymbol{x}_i.$$

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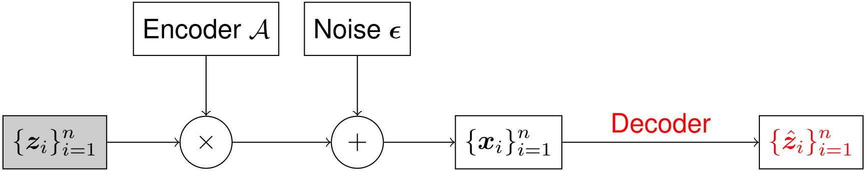
# Typical Inverse Problems




- The observation model can be represented as:

$$x_i = \mathcal{A}(z_i) + \epsilon, \quad i = 1, \ldots, n$$

- For known encoder $\mathcal{A}$ and observations $\{x_i\}_{i=1}^n$, wish to train a decoder.

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# Empirical Bayes approach

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

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

- **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:

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

# $G$-modelling for Empirical Bayes

Estimation:

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

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!

# $G$-modelling for Empirical Bayes

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Intractable for complicated prior distribution or high dimension latent space!

# Evidence Lower Bound

## Lemma: Variational Lower Bound

$$\begin{aligned}\log p(\boldsymbol{x}) &\geq \mathbb{E}_{\boldsymbol{z}\sim q}[\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z})] \\ &\triangleq \mathbb{E}_{\boldsymbol{z}\sim q}[\log p(\boldsymbol{z}) + \log p(\boldsymbol{x} \mid \boldsymbol{z}) - \log q(\boldsymbol{z})]\end{aligned}$$

Proof.

$$\begin{aligned}\log p(\boldsymbol{x}) &= \log \int_{\boldsymbol{z}} p(\boldsymbol{x}, \boldsymbol{z})\, \mathrm{d}\boldsymbol{z} \\ &= \log \int_{\boldsymbol{z}} p(\boldsymbol{x}, \boldsymbol{z}) \frac{q(\boldsymbol{z})}{q(\boldsymbol{z})}\, \mathrm{d}\boldsymbol{z} = \log \left( \mathbb{E}_{\boldsymbol{z}\sim q}\left[ \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q(\boldsymbol{z})} \right] \right) \\ &\geq \mathbb{E}_{\boldsymbol{z}\sim q}\left[ \log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q(\boldsymbol{z})} \right] = \mathbb{E}_{\boldsymbol{z}\sim q}[\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z})]\end{aligned}$$

□

# Variational Inference Approach

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

- 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.

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# Vanilla Amortized Variational Inference

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

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

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

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

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

# Vanilla Amortized Variational Inference

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  where:

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  Optimize for $\boldsymbol{\Lambda}$: parametric optimization techniques.

# Vanilla Amortized Variational Inference (AVI)

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

**Input:** $\{\boldsymbol{x}_i\}_{i=1}^{n}$, $p(\boldsymbol{x} \mid \boldsymbol{z})$, $\eta$, and $n_{\text{critic}}$, the number of iterations of the $\phi$ update per $\boldsymbol{\Lambda}$ estimation.
**Output:** $\hat{\boldsymbol{\Lambda}}, \hat{\phi}$: learnt parameters.

1: $\hat{\boldsymbol{\Lambda}}, \hat{\phi} \leftarrow$ initialize parameters
2: **for** $t = 0, \ldots, n_{\text{critic}}$ **do**
3: Generate $\{z_{(i)}\}_{i=1}^{B}$ by the reparameriation trick.
4: Compute the objective function $\tilde{L}_{\boldsymbol{\Lambda},\boldsymbol{\phi}}$ and its gradients:

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

5: Update $\hat{\phi}$ using Adam optimizer
6: **end for**
7: Generate $\{z_{(i)}\}_{i=1}^{B}$, and update $\boldsymbol{\Lambda}$ by optimizing $\sum_{i=1}^{B} \log(\boldsymbol{z}_{(i)}; \boldsymbol{\Lambda})$.

# AVI with Inverse Autoregressive Flow

- Vanilla AVI suffices from the inexact approximation posterior.

## Inverse Autoregressive Flow Trick

Initialize with

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

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

# AVI with Inverse Autoregressive Flow

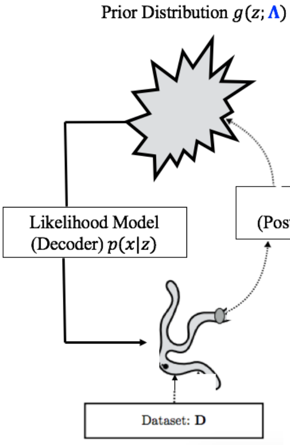
Two things to be modified based on Vanilla AVI:

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

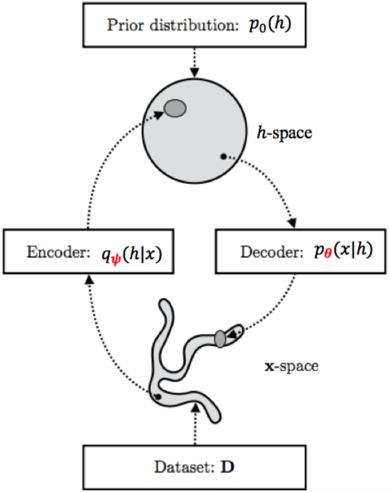
1. The sampling for $\boldsymbol{z}$ via $q_\phi(\boldsymbol{z}_i \mid \boldsymbol{x}_i)$ follows Inverse Autoregressive Flow process;
2. Substitute the evaluation for the term $\log q_\phi(\boldsymbol{z}_i \mid \boldsymbol{x}_i)$:

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

# Connection to VAE




$g(z;\Lambda) = G_\theta \# p_0(h)$



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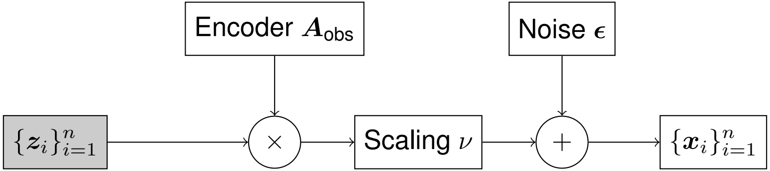
# Problem Setting




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

where $\nu$ is the sigmoid function.

# Vanilla AVI Approach

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

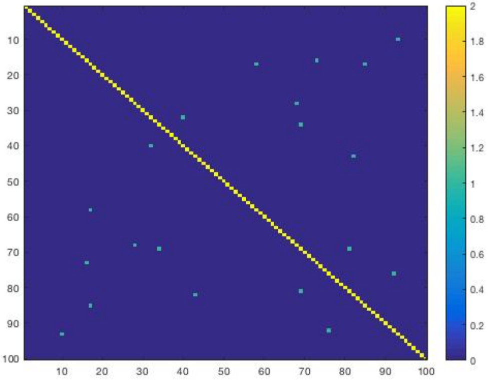
$$\frac{1}{2}\,\text{Trace}\left(\boldsymbol{\Lambda}\cdot\sum_{i=1}^{B}(\boldsymbol{z}_{(i)})(\boldsymbol{z}_{(i)})^{\mathrm{T}}\right)+\frac{1}{2\sigma_{\text{obs}}^2}\sum_{i=1}^{B}\|\boldsymbol{x}_{(i)}-\nu(\boldsymbol{A}_{\text{obs}}\boldsymbol{z}_{(i)})\|^2-\sum_{i=1,j}^{B}\log|\sigma_{(i),j}|$$

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

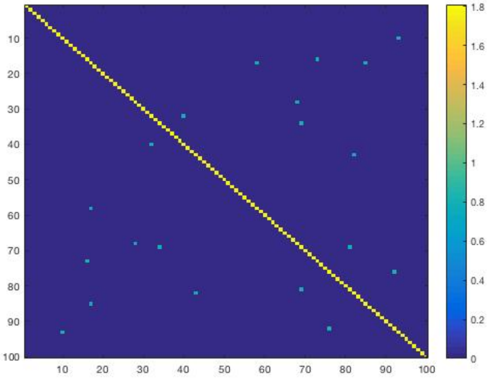
$$\arg\max_{\boldsymbol{\Lambda}}\quad -\lambda\cdot\|\boldsymbol{\Lambda}\|_{\ell_1,\text{off}}+\frac{B}{2}\log|\boldsymbol{\Lambda}|-\frac{B}{2}\,\text{Trace}\left[\boldsymbol{\Lambda}\cdot\frac{1}{B}\sum_{i=1}^{B}(\boldsymbol{z}_{(i)})(\boldsymbol{z}_{(i)})^{\mathrm{T}}\right]$$

Disadvantage: graphical lasso problem is computationally expansive!

# Simulation Results

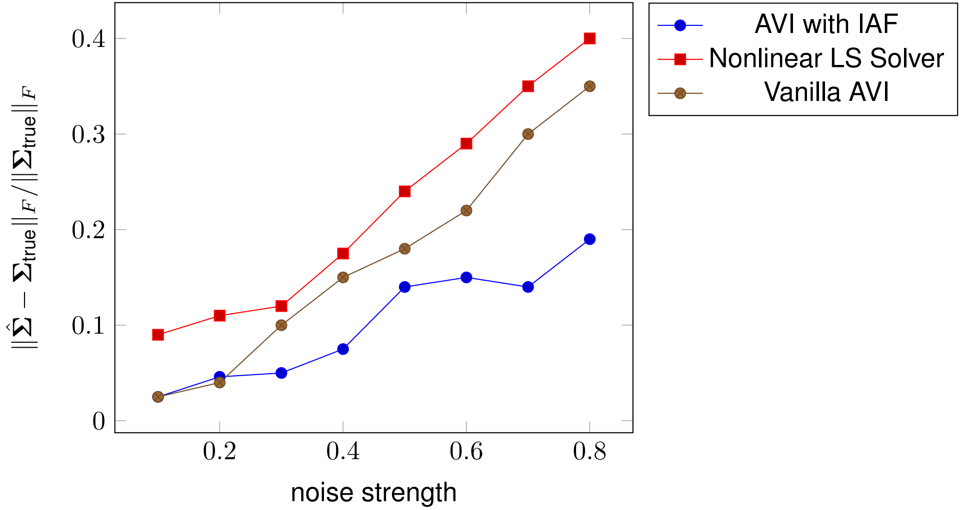



(a) Underlying Precision matrix $\mathbf{\Lambda}_{\text{true}}$




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

# Simulation Results



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# Conclusion

- The inverse problem is solved by amoritzed variational inference with IAF trick:

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

  This approach is to jointly estimating $g(\boldsymbol{z})$ and $p(\boldsymbol{z} \mid \boldsymbol{x})$.
- Applicable to general prior and likelihood model.
- Sub-optimality gap and Generalization bound is still open.

# Acknowledgement

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