From Statistical Estimation and Generative Modeling to Inverse Problems

LECTURE 5: INVERSE PROBLEMS

Inverse Problems

- Problem Definition
- Early Efforts
- Solutions Based on GANs
 - Add-Hoc
 - Applying Statistical Estimation
- Examples

Problem Definition

We are given vector X (measurements) and interested in estimating vector Y

We assume X = T(Y) + W where T(Y) general (mostly) known transformation

Basic characteristic: $\dim(X) \leq \dim(Y)$



Image Separation



Early Efforts

Inpainting





Diffusion based inpainting



No prior information, training data not very useful

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Solutions Based on GANs

Available training data $\{X_1, \dots, X_n\}$

Design generator G(Z) so that when applied to Z with $Z \sim h(Z)$ then Y = G(Z) has same density as training data Generate $\{Z_1, ..., Z_m\}$ with density h(Z)

$$\hat{\mathsf{J}}(\theta,\vartheta) = \frac{1}{n} \sum_{t=1}^{n} \phi \big(\mathsf{D}(X_t,\vartheta) \big) + \frac{1}{m} \sum_{t=1}^{m} \psi \big(\mathsf{D}\big(\mathsf{G}(Z_t,\theta),\vartheta\big) \big)$$

Discriminator

$$\min_{\theta} \max_{\vartheta} \hat{\mathsf{J}}(\theta,\vartheta)$$

Assume known Generative Model {G(Z),h(Z)}, also Discriminator D(X)

General Problem

Given vector X (measurements) we are interested in estimating vector Y with X = T(Y)+W and T(Y) known transformation

Y follows Generative Model

There exists Z following density h(Z) such that Y = G(Z)Instead of estimating Y from X we estimate input to generative model Z



Measurements X = T(Y) + WCompute estimate \hat{Y} Measurements X = T(G(Z)) + WCompute estimate \hat{Z} and let $\hat{Y} = G(\hat{Z})$

Since $\dim(Z) \ll \dim(Y)$

Significant computational gain and more stable processing Select \hat{Z} so that measurements X and $T(G(\hat{Z}))$ are "close"

$$\min_{Z} \|X - \mathsf{T}\big(\mathsf{G}(Z)\big)\|^2 \implies \hat{Z} = \arg\min_{Z} \|X - \mathsf{T}\big(\mathsf{G}(Z)\big)\|^2$$

Well defined optimization, computationally stable

Doesn't Work!!

$$\begin{split} \hat{Y} &= \mathsf{G}(\hat{Z}) \ \text{does not have the correct characteristics} \\ \text{Recall that generative model is the pair } \{\mathsf{G}(Z),\mathsf{h}(Z)\} \\ &\quad \text{Even if } \mathsf{T}\big(\mathsf{G}(\hat{Z})\big) \ \text{"close" to } X \text{, if likelihood } \mathsf{h}(\hat{Z}) \ll 1 \\ &\quad \text{then } \hat{Y} = \mathsf{G}(\hat{Z}) \text{ is "bad" result} \end{split}$$

Must take into account input density $\mathsf{h}(Z)$

Ad-Hoc Solutions

Yeh et al. (2017), (2018)

Assumes generative model trained with cross entropy method

$$\phi(z) = \log(1-z), \ \psi(z) = \log(z), \ z \in (0,1) \Rightarrow$$

Design G(Z) generator, D(Z) discriminator, when $Z \sim h(Z)$





To tune parameter λ need ideal images $\{Y_1, ..., Y_n\}$ apply transformation $X_i = T(Y_i)$ For various values of λ for each $\{X_1, ..., X_n\}$ compute

$$\begin{split} \hat{Z}_1(\lambda), \dots, \hat{Z}_n(\lambda) &\Rightarrow \hat{Y}_1(\lambda), \dots, \hat{Y}_n(\lambda) \qquad \lambda_i = \arg\min_{\lambda} \|Y_i - \hat{Y}_i(\lambda)\| \\ \lambda &= \frac{1}{n} \{\lambda_1 + \dots + \lambda_n\} \end{split}$$
Requires exact knowledge of T(Y)

Asim et al. (2019)

$$\hat{Z} = \arg \min_{Z} \left\{ \|X - \mathsf{T}(\mathsf{G}(Z))\|^{2} - \lambda \log(\mathsf{h}(Z)) \right\}$$
Parameter needs tuning



Requires exact knowledge of T(Y)

Siavelis et al. (2020)

$$\hat{Z} = \arg\min_{Z} \left\{ \|X - \mathsf{T}\big(\mathsf{G}(Z)\big)\|_{L_{1}} - \lambda\Big(1 - \mathsf{D}\big(\mathsf{G}(Z)\big)\Big) \right\}$$

Parameter needs tuning





Requires exact knowledge of T(Y)

Applying Statistical Estimation

Given densities f(X|Z) and prior h(Z), for measurement X estimate Z MAP estimator is of the form

$$\hat{Z} = \arg \max_{Z} \mathsf{f}(Z|X) = \arg \max_{Z} \mathsf{f}(X,Z) = \arg \max_{Z} \mathsf{f}(X|Z)\mathsf{h}(Z)$$

Let $Z = \{Z_1, Z_2\}$ where there is prior for Z_1 but not for Z_2 Treat non-existing prior as degenerate uniform

$$\begin{aligned} \arg\max_{Z_1,Z_2} f(Z_1,Z_2|X) &= \arg\max_{Z_1,Z_2} f(X,Z_1,Z_2) \\ &= \arg\max_{Z_1,Z_2} f(X|Z_1,Z_2)h(Z_1,Z_2) \\ &= \arg\max_{Z_1,Z_2} f(X|Z_1,Z_2)h_1(Z_1|Z_2)h_2(Z_2) \\ h_2(Z_2) \text{ degenerate uniform } &= \arg\max_{Z_1,Z_2} f(X|Z_1,Z_2)h_1(Z_1|Z_2) \end{aligned}$$

If interested in estimating Z_1 and Z_2 are nuisance parameters then

$$\hat{Z}_1 = \arg \max_{Z_1} \left\{ \max_{Z_2} f(X|Z_1, Z_2) h_1(Z_1|Z_2) \right\}$$

where $\mathbf{h}_1(Z_1 \, | \, Z_2)$ prior of Z_1 given Z_2

If Z_1 does not depend on Z_2 then $\mathsf{h}_1(Z_1 \, | \, Z_2) = \mathsf{h}_1(Z_1)$ and

$$\hat{Z}_1 = \arg \max_{Z_1} \left\{ \max_{Z_2} \mathsf{f}(X|Z_1, Z_2) \mathsf{h}_1(Z_1) \right\}$$

We are given vector X (measurements) and interested in estimating vector Y

We assume $X = T(Y, \alpha) + W = T(G(Z), \alpha) + W$

 $T(Y, \alpha)$: transformation of known mathematical form possibly containing unknown parameters α . Can be different per measurement X

W: additive noise with density $g_w(W, \beta)$ possibly containing unknown parameters β . Can be different per measurement *X*

Z: follows density h(Z) from generative model {G(Z), h(Z)}

$$\begin{split} Z_1 = & Z, \quad Z_2 = \{ \alpha, \beta \} \quad \mathsf{f}(X|Z_1, Z_2) = \mathsf{f}(X|Z, \alpha, \beta) = \mathsf{g}_w \Big(X - \mathsf{T}\big(\mathsf{G}(Z), \alpha\big), \beta \Big) \\ \hat{Z} = \arg \max_Z \Big\{ \max_{\alpha, \beta} \mathsf{f}(X|Z, \alpha, \beta) \mathsf{h}(Z) \Big\} \\ = \arg \max_Z \Big\{ \max_{\alpha, \beta} \mathsf{g}_w \Big(X - \mathsf{T}\big(\mathsf{G}(Z), \alpha\big), \beta \Big) \mathsf{h}(Z) \Big\} \end{split}$$

$$\hat{Z} = \arg \max_{Z} \Big\{ \max_{\alpha} \max_{\beta} \mathsf{g}_{w} \Big(X - \mathsf{T} \big(\mathsf{G}(Z), \alpha \big), \beta \Big) \mathsf{h}(Z) \Big\}$$

W: additive noise is Gaussian mean 0 and covariance $\beta^2 I$

$$\begin{split} \max_{\beta} \mathsf{g}_w \Big(X - \mathsf{T}\big(\mathsf{G}(Z), \alpha\big), \beta \Big) &= \max_{\beta} \frac{e^{-\|X - \mathsf{T}(\mathsf{G}(Z), \alpha)\|^2 / 2\beta^2}}{(\sqrt{2\pi\beta^2})^N} \\ &= \frac{\mathsf{C}}{\|X - \mathsf{T}(\mathsf{G}(Z), \alpha)\|^N} \qquad N: \text{length of measurement vector } X \\ \hat{Z} &= \arg\max_{Z} \left\{ \max_{\alpha} \frac{\mathsf{C}\,\mathsf{h}(Z)}{\|X - \mathsf{T}(\mathsf{G}(Z), \alpha)\|^N} \right\} \\ &= \arg\max_{Z} \frac{\mathsf{h}(Z)}{(\min_{\alpha} \|X - \mathsf{T}(\mathsf{G}(Z), \alpha)\|^2)^{N/2}} \end{split}$$

Z: If input of generative model is Gaussian with mean 0 and covariance identity

$$\hat{Z} = \arg \max_{Z} \frac{\mathsf{C}' \, e^{-\|Z\|^2/2}}{(\min_{\alpha} \|X - \mathsf{T}(\mathsf{G}(Z), \alpha)\|^2)^{N/2}}$$

$$\hat{Z} = \arg\min_{Z} \left\{ \log \left(\min_{\alpha} \|X - \mathsf{T}(\mathsf{G}(Z), \alpha)\|^2 \right) + \frac{1}{N} \|Z\|^2 \right\}$$

$$\Leftrightarrow \min_{Z,\alpha} \left\{ \log \left(\|X - \mathsf{T}(\mathsf{G}(Z),\alpha)\|^2 \right) + \frac{1}{N} \|Z\|^2 \right\}$$

If transformation satisfies

$$\mathsf{T}(Y,\alpha) = \alpha_1 \mathsf{T}_1(Y) + \dots + \alpha_m \mathsf{T}_m(Y)$$

then $\mathsf{T}(\mathsf{G}(Z),\alpha) = \alpha_1 \mathsf{T}_1(\mathsf{G}(Z)) + \dots + \alpha_m \mathsf{T}_m(\mathsf{G}(Z)) = \mathfrak{G}(Z)A$

where
$$\mathcal{G}(Z) = \begin{bmatrix} \mathsf{T}_1(\mathsf{G}(Z)) \cdots \mathsf{T}_m(\mathsf{G}(Z)) \end{bmatrix}, A = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_m \end{bmatrix}$$

$$\begin{split} \min_{A} \|X - \mathcal{G}(Z)A\|^2 &= \|X\|^2 - X^{\mathsf{T}}\mathcal{G}(Z) \big(\mathcal{G}^{\mathsf{T}}(Z)\mathcal{G}(Z)\big)^{-1} \mathcal{G}^{\mathsf{T}}(Z)X\\ \hat{Z} &= \arg\min_{Z} \left\{ \log \Big(\|X\|^2 - X^{\mathsf{T}}\mathcal{G}(Z) \big(\mathcal{G}^{\mathsf{T}}(Z)\mathcal{G}(Z)\big)^{-1} \mathcal{G}^{\mathsf{T}}(Z)X\Big) + \frac{1}{N} \|Z\|^2 \right\} \end{split}$$

Examples



No parameters to tune

De-Quantization

2 levels per RGB channel, 8 colors



De-Quantization

3 levels per RGB channel, 27 colors



De-Quantization

5 levels per RGB channel, 125 colors



De-Quantization and Colorization

 $RGB \rightarrow Gray \rightarrow BW (2 levels)$



With threshold estimation

Data Mixtures

We assume two independent data vectors Y_1 , Y_2 that are combined as

$$X = \alpha_1 Y_1 + \alpha_2 Y_2 + W$$

From mixture X recover original $Y_{\rm 1}$, $Y_{\rm 2}$

- Y_1 : generative model {G₁(Z₁),h₁(Z₁)}
- Y_2 : generative model {G $_2(Z_2), \mathsf{h}_2(Z_2)$ }

 $W\!\!:$ additive noise with density $\,{\bf g}_w(W,\!\beta)$ containing unknown parameters β If W Gaussian, mean 0, covariance $\,\beta^2 I$

If inputs of both generative models Gaussian, mean 0, covariance identity

$$\{ \hat{Z}_1, \hat{Z}_2 \} = known$$
arg min
$$\sum_{Z_1, Z_2} \left\{ \log \left(\|X - \alpha_1 \mathsf{G}_1(Z_1) - \alpha_2 \mathsf{G}_2(Z_2)\|^2 \right) + \frac{1}{N} \left(\|Z_1\|^2 + \|Z_2\|^2 \right) \right\}$$

$$\begin{split} &\{\hat{Z}_1, \hat{Z}_2\} = & \text{unknown} \\ & \text{arg } \min_{Z_1, Z_2} \left\{ \log \left(\min_{\alpha_1, \alpha_2} \|X - \alpha_1 \mathsf{G}_1(Z_1) - \alpha_2 \mathsf{G}_2(Z_2)\|^2 \right) + \frac{1}{N} \left(\|Z_1\|^2 + \|Z_2\|^2 \right) \right\} \\ & = \arg \min_{Z_1, Z_2} \left\{ \log \left(\|X\|^2 - X^\intercal \mathfrak{G}(Z_1, Z_2) \left(\mathfrak{G}^\intercal(Z_1, Z_2) \mathfrak{G}(Z_1, Z_2) \right)^{-1} \mathfrak{G}^\intercal(Z_1, Z_2) X \right) \\ & \quad + \frac{1}{N} \left(\|Z_1\|^2 + \|Z_2\|^2 \right) \right\} \\ & \text{where } \quad \mathfrak{G}(Z_1, Z_2) = \left[\mathsf{G}_1(Z_1) \mathsf{G}_2(Z_2) \right] \end{split}$$

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Known coefs Uknown coefs



Known coefs Uknown coefs



Nonlinear Data Mixtures

We assume two independent data vectors Y_1 , Y_2 that are combined as

$$X = \mathsf{T}(Y_1, Y_2, \alpha) + W$$

 $Y_1:$ generative model {G $_1(Z_1), \mathsf{h}_1(Z_1)$ }

 Y_2 : generative model {G $_2(Z_2), h_2(Z_2)$ }

W: additive noise with density $g_w(W,\beta)$ containing unknown parameters β

$$\begin{aligned} &\{\hat{Z}_{1}, \hat{Z}_{2}\} = \\ &\arg\min_{Z_{1}, Z_{2}} \left\{ \log\left(\min_{\alpha} \|X - \mathsf{T}\big(\mathsf{G}_{1}(Z_{1}), \mathsf{G}_{2}(Z_{2}), \alpha\big)\|^{2}\big) + \frac{1}{N}\big(\|Z_{1}\|^{2} + \|Z_{2}\|^{2}\big) \right\} \\ &\Rightarrow \min_{Z_{1}, Z_{2}, \alpha} \left\{ \log\big(\|X - \mathsf{T}\big(\mathsf{G}_{1}(Z_{1}), \mathsf{G}_{2}(Z_{2}), \alpha\big)\|^{2}\big) + \frac{1}{N}\big(\|Z_{1}\|^{2} + \|Z_{2}\|^{2}\big) \right\} \end{aligned}$$