Regularization of Inverse Problems

Matthias J. Ehrhardt

January 28, 2019
What is an Inverse Problem?

- $A : \mathcal{U} \rightarrow \mathcal{V}$ mapping between Hilbert spaces $\mathcal{U}, \mathcal{V}$, $A \in L(\mathcal{U}, \mathcal{V})$
- physical model $A$, cause $u$ and effect $A(u) = Au$.

**Direct / Forward Problem:** given $u$, calculate $Au$. 
What is an Inverse Problem?

- $A : \mathcal{U} \rightarrow \mathcal{V}$ mapping between Hilbert spaces $\mathcal{U}, \mathcal{V}$, $A \in L(\mathcal{U}, \mathcal{V})$
- physical model $A$, cause $u$ and effect $A(u) = Au$.

**Direct / Forward Problem**: given $u$, calculate $Au$.

- Example 1: ray transform (used in CT, PET, ...)

$$A : L^2(\Omega) \rightarrow L^2([0, 2\pi], [-1, 1]), \quad Au(\theta, s) = \int_{\mathbb{R}} u(s\theta + t\theta^\perp) dt$$
What is an Inverse Problem?

- \( A : \mathcal{U} \rightarrow \mathcal{V} \) mapping between Hilbert spaces \( \mathcal{U}, \mathcal{V} \), \( A \in L(\mathcal{U}, \mathcal{V}) \)
- physical model \( A \), cause \( u \) and effect \( A(u) = Au \).

**Direct / Forward Problem**: given \( u \), calculate \( Au \).

- Example 1: ray transform (used in CT, PET, ...)

\[
A : L^2(\Omega) \rightarrow L^2([0, 2\pi], [-1, 1]), \quad Au(\theta, s) = \int_{\mathbb{R}} u(s\theta + t\theta^\perp) dt
\]
What is an Inverse Problem?

- A mapping between Hilbert spaces $\mathcal{U}, \mathcal{V}$, $A \in L(\mathcal{U}, \mathcal{V})$
- Physical model $A$, cause $u$ and effect $A(u) = Au$.

**Direct / Forward Problem**: given $u$, calculate $Au$.

Example 1: ray transform (used in CT, PET, ...)

$$A : L^2(\Omega) \rightarrow L^2([0, 2\pi], [-1, 1]), \quad Au(\theta, s) = \int_{\mathbb{R}} u(s\theta + t\theta^\perp) dt$$
What is an Inverse Problem?

- $A : \mathcal{U} \rightarrow \mathcal{V}$ mapping between Hilbert spaces $\mathcal{U}, \mathcal{V}$, $A \in L(\mathcal{U}, \mathcal{V})$
- physical model $A$, cause $u$ and effect $A(u) = Au$.

**Direct / Forward Problem**: given $u$, calculate $Au$.

- Example 1: ray transform (used in CT, PET, ...)

$$A : L^2(\Omega) \rightarrow L^2([0, 2\pi], [-1, 1]), \quad Au(\theta, s) = \int_{\mathbb{R}} u(s\theta + t\theta^\perp) \, dt$$

**Inverse Problem**: Given $v$, calculate $u$ with $Au = v$.

Infer from the effect the cause.
What is the problem with Inverse Problems?

**Examples**
A solution may

- not exist. $Au = 0$, $v \neq 0$
What is the problem with Inverse Problems?

Examples
A solution may

- not exist. \( Au = 0, v \neq 0 \)
- not be unique. \( Au = 0, v = 0 \)
What is the problem with Inverse Problems?

Examples

A solution may

- **not exist.** $Au = 0, v \neq 0$
- **not be unique.** $Au = 0, v = 0$
- **be sensitive to noise.**
  - Positron Emission Tomography (PET)
  - Data: PET scanner in London
  - Model: ray transform, $Au(L) = \int_L u(r)dr$
  - Find $u$ such that $Au = v$
What is the problem with Inverse Problems?

Examples
A solution may

▶ **not exist.** \( Au = 0, v \neq 0 \)
▶ **not be unique.** \( Au = 0, v = 0 \)
▶ **be sensitive to noise.**
  - Positron Emission Tomography (PET)
  - Data: PET scanner in London
  - Model: ray transform, \( Au(L) = \int_L u(r)dr \)
  - Find \( u \) such that \( Au = v \)
What is the problem with Inverse Problems?

Definition (Jacques Hadamard, 1865-1963): An Inverse Problem “$Au = v$” is called well-posed, if the solution

(1) exists.
(2) is unique.
(3) depends continuously on the data.

“Small errors in $v$ lead to small errors in $u$.”

Otherwise, we call it ill-posed.
What is the problem with Inverse Problems?

**Definition** (Jacques Hadamard, 1865-1963):
An Inverse Problem \( Au = v \) is called **well-posed**, if the solution

1. exists.
2. is **unique**.
3. depends **continuously** on the data.
   “Small errors in \( v \) lead to small errors in \( u \).”

Otherwise, we call it **ill-posed**.

Almost all interesting inverse problems are ill-posed.
Definition: Let $v \in \mathcal{V}$. The set of all approximate solutions of 
“$Au = v$” is

$$
\mathcal{L} := \left\{ u \in \mathcal{U} \mid \|Au - v\| \leq \|Az - v\| \quad \forall z \in \mathcal{U} \right\}.
$$

If a solution $z \in \mathcal{U}$ exists, $\|Az - v\| = 0$, then

$$
\mathcal{L} = \left\{ u \in \mathcal{U} \mid Au = v \right\}.
$$
Generalized Solutions

**Definition:** Let $v \in \mathcal{V}$. The set of all approximate solutions of 
"$Au = v$" is

$$
\mathcal{L} := \left\{ u \in \mathcal{U} \mid \|Au - v\| \leq \|Az - v\| \quad \forall z \in \mathcal{U} \right\}.
$$

If a solution $z \in \mathcal{U}$ exists, $\|Az - v\| = 0$, then

$$
\mathcal{L} = \left\{ u \in \mathcal{U} \mid Au = v \right\}
$$

**Definition:** An approximate solution $\bar{u} \in \mathcal{L}$ is called a **minimal-norm-solution**, if

$$
\|\bar{u}\| \leq \|u\| \quad \forall u \in \mathcal{L}.
$$
Properties of Minimal-Norm-Solutions

Recall:

- Range / image of $A$: $\mathcal{R}_A := \{ v \in \mathcal{V} \mid \exists u \in \mathcal{U} \ Au = v \}$
- Orthogonal complement: $\mathcal{A}^\perp := \{ v \in \mathcal{V} \mid \langle v, z \rangle = 0 \ \forall z \in \mathcal{A} \}$
- Minkowski sum: $\mathcal{A} + \mathcal{B} := \{ u + v \mid u \in \mathcal{A}, v \in \mathcal{B} \}$
Properties of Minimal-Norm-Solutions

Recall:

- Range / image of $A$: $\mathcal{R}_A := \{ v \in \mathcal{V} \mid \exists u \in \mathcal{U} \ Au = v \}$
- Orthogonal complement: $\mathcal{A}^\perp := \{ v \in \mathcal{V} \mid \langle v, z \rangle = 0 \ \forall z \in \mathcal{A} \}$
- Minkowski sum: $\mathcal{A} + \mathcal{B} := \{ u + v \mid u \in \mathcal{A}, v \in \mathcal{B} \}$

**Proposition:** $\mathcal{R}_A$ is closed if and only if $\mathcal{R}_A + \mathcal{R}_A^\perp = \mathcal{V}$. 
Properties of Minimal-Norm-Solutions

Recall:

- Range / image of $A$: $\mathcal{R}_A := \{ v \in \mathcal{V} \mid \exists u \in \mathcal{U} \ Au = v \}$
- Orthogonal complement: $\mathcal{A}^\perp := \{ v \in \mathcal{V} \mid \langle v, z \rangle = 0 \ \forall z \in \mathcal{A} \}$
- Minkowski sum: $\mathcal{A} + \mathcal{B} := \{ u + v \mid u \in \mathcal{A}, v \in \mathcal{B} \}$

**Proposition:** $\mathcal{R}_A$ is closed if and only if $\mathcal{R}_A + \mathcal{R}_A^\perp = \mathcal{V}$.

**Example:** $A : \ell^2 \to \ell^2$, $(Au)_j = \frac{u_j}{j}$. Range $\mathcal{R}_A$ not closed.
Properties of Minimal-Norm-Solutions

Recall:

- Range / image of $A$: $\mathcal{R}_A := \{ v \in \mathcal{V} \mid \exists u \in \mathcal{U} \ Au = v \}$
- Orthogonal complement: $A^\perp := \{ v \in \mathcal{V} \mid \langle v, z \rangle = 0 \ \forall z \in A \}$
- Minkowski sum: $A + B := \{ u + v \mid u \in A, v \in B \}$

Proposition: $\mathcal{R}_A$ is closed if and only if $\mathcal{R}_A + \mathcal{R}_{A}^\perp = \mathcal{V}$.

Example: $A : \ell^2 \rightarrow \ell^2, (Au)_j = \frac{u_j}{j}$. Range $\mathcal{R}_A$ not closed.

Theorem: Let $v \in \mathcal{R}_A + \mathcal{R}_{A}^\perp$. Then there exists a unique minimal-norm-solution $\overline{u}$ of “$Au = v$”. We write $A^\dagger v = \overline{u}$. 
Properties of Minimal-Norm-Solutions

Recall:
- Range / image of $A$: $\mathcal{R}_A := \{ v \in \mathcal{V} \mid \exists u \in \mathcal{U} \; Au = v \}$
- Orthogonal complement: $A^\perp := \{ v \in \mathcal{V} \mid \langle v, z \rangle = 0 \; \forall z \in A \}$
- Minkowski sum: $A + B := \{ u + v \mid u \in A, \; v \in B \}$

**Proposition:** $\mathcal{R}_A$ is closed if and only if $\mathcal{R}_A + \mathcal{R}_A^\perp = \mathcal{V}$.

**Example:** $A : \ell^2 \to \ell^2, (Au)_j = \frac{u_j}{j}$. Range $\mathcal{R}_A$ not closed.

**Theorem:** Let $v \in \mathcal{R}_A + \mathcal{R}_A^\perp$. Then there exists a unique minimal-norm-solution $\bar{u}$ of “$Au = v$”. We write $A^\dagger v = \bar{u}$.

**Theorem:** If $\mathcal{R}_A$ is not closed, then $\bar{u}$ does not depend continuously on $v$, i.e. $A^\dagger$ is not continuous.
Regularization

\[ \overline{u} = A^\dagger v \]

Definition: A family \( \{ R_{\alpha} \} \) is called regularization of \( A^\dagger \), if for all \( \alpha > 0 \) the mapping \( R_{\alpha} : \mathcal{V} \to \mathcal{U} \) is continuous.
Regularization

\[ \bar{u} = A^\dagger v \]

Definition: A family \( \{ R_\alpha \} \) for all \( \alpha > 0 \) is called regularization of \( A^\dagger \), if for all \( v \in \mathbb{R}^A + R^\perp_A \) \( \lim_{\alpha \to 0} R_\alpha v = A^\dagger v \).
Definition: A family \( \{ R_\alpha \} \) is called regularization of \( A^\dagger \), if for all \( \alpha > 0 \) the mapping \( R_\alpha : V \to U \) is continuous.

\[
\begin{align*}
\overline{u} &= A^\dagger v \\
R_\alpha v^\delta &= A^\dagger v \\
A^\dagger v^\delta &= v^\delta
\end{align*}
\]
Definition: A family \( \{ R_\alpha \}_{\alpha > 0} \) is called regularization of \( A^\dagger \), if

- for all \( \alpha > 0 \) the mapping \( R_\alpha : \mathcal{V} \rightarrow \mathcal{U} \) is continuous.
- for all \( v \in \mathcal{R}_A + \mathcal{R}_A^\perp \) \( \lim_{\alpha \rightarrow 0} R_\alpha v = A^\dagger v \).
Definition: A family \( \{ R_\alpha \}_{\alpha > 0} \) is called regularization of \( A^\dagger \), if

- for all \( \alpha > 0 \) the mapping \( R_\alpha : \mathcal{V} \rightarrow \mathcal{U} \) is continuous.
- for all \( v \in \mathcal{R}_A + \mathcal{R}_A^\perp \) \( \lim_{\alpha \rightarrow 0} R_\alpha v = A^\dagger v \).
Regularization

Definition: A family \( \{ R_\alpha \}_{\alpha > 0} \) is called regularization of \( A^\dagger \), if

\[ \text{for all } \alpha > 0 \text{ the mapping } R_\alpha : \mathcal{V} \to \mathcal{U} \text{ is continuous.} \]

\[ \text{for all } v \in \mathcal{R}_A + \mathcal{R}_A^\perp \lim_{\alpha \to 0} R_\alpha v = A^\dagger v. \]
Popular examples of regularization

**Tikhonov regularization**
(Andrey Tikhonov, 1906-1993)

\[ R_{\alpha}v^\delta = \operatorname{arg\ min}_u \left\{ \| Au - v^\delta \|^2 + \alpha \| u \|^2 \right\} \]
Popular examples of regularization

**Tikhonov regularization**
(Andrey Tikhonov, 1906-1993)

\[ R_{\alpha}v^\delta = \arg \min_u \left\{ \|Au - v^\delta\|^2 + \alpha \|u\|^2 \right\} \]

\[ = (A^* A + \alpha I)^{-1} A^* v^\delta \]
Popular examples of regularization

**Tikhonov regularization**
(Andrey Tikhonov, 1906-1993)

\[
R_\alpha \nu^\delta = \arg \min_u \left\{ \|Au - \nu^\delta\|^2 + \alpha \|u\|^2 \right\}
= (A^*A + \alpha I)^{-1} A^* \nu^\delta
\]

**Proposition:** \((A^*A + \alpha I)^{-1} \in L(U,U)\) for all \(\alpha > 0\)
Popular examples of regularization

**Tikhonov regularization**
(Andrey Tikhonov, 1906-1993)

\[
R_{\alpha} \nu^\delta = \arg \min_u \left\{ \| Au - \nu^\delta \|^2 + \alpha \| u \|^2 \right\} = (A^* A + \alpha I)^{-1} A^* \nu^\delta
\]

**Proposition:** \((A^* A + \alpha I)^{-1} \in L(U, \mathcal{U})\) for all \(\alpha > 0\)

**Variational regularization**

\[
R_{\alpha} \nu^\delta = \arg \min_u \left\{ D(Au, \nu^\delta) + \alpha J(u) \right\}
\]

- **data fit** \(D\): “divergence” \(D(x, y) \geq 0, D(x, y) = 0\) iff \(x = y\)
  Examples: \(D(x, y) = \|x - y\|^2, \|x - y\|_1, \int x - y + y \log(y/x)\)

- **regularizer** \(J\): Penalizes unwanted features; ensures stability
  Examples: \(J(u) = \|u\|^2, \|u\|_1, \text{TV}(u) = \|\nabla u\|_1\)
Popular examples of regularization

**Tikhonov regularization**
(Andrey Tikhonov, 1906-1993)

\[ R_\alpha \nu^\delta = \arg \min_u \left\{ \|Au - \nu^\delta\|^2 + \alpha\|u\|^2 \right\} \]
\[ = (A^*A + \alpha I)^{-1}A^*\nu^\delta \]

**Proposition:** \((A^*A + \alpha I)^{-1} \in L(U,U)\) for all \(\alpha > 0\)

**Variational regularization**

\[ R_\alpha \nu^\delta = \arg \min_u \left\{ D(Au, \nu^\delta) + \alpha J(u) \right\} \]

- **data fit** \(D\): “divergence” \(D(x, y) \geq 0, D(x, y) = 0\) iff \(x = y\)
  Examples: \(D(x, y) = \|x - y\|^2, \|x - y\|_1, \int x - y + y \log(y/x)\)

- **regularizer** \(J\): Penalizes unwanted features; ensures stability
  Examples: \(J(u) = \|u\|^2, \|u\|_1, \text{TV}(u) = \|\nabla u\|_1\)

- **decouples solution of inverse problem into 2 steps:**
  1. **Modelling:** choose \(D, J, A, \alpha\).
  2. **Optimization:** connection to statistics, machine learning ...
Summary

▶ **Inverse problems**
  ▶ forward / direct problem
  ▶ ill-posedness; interesting inverse problems are ill-posed
  ▶ generalized solutions, minimal-norm-solution

▶ **Regularization**
  ▶ stable approximation of minimal-norm-solution
  ▶ Tikhonov regularization
  ▶ variational regularization