PERSONAL NOTES

INVERSE PROBLEMS

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2023

Class 1

$$\text{cause} \leftarrow \boxed{m(\vec{x},t;\theta)} \leftarrow \text{effect}.$$

* - sparely measured.

noisy.

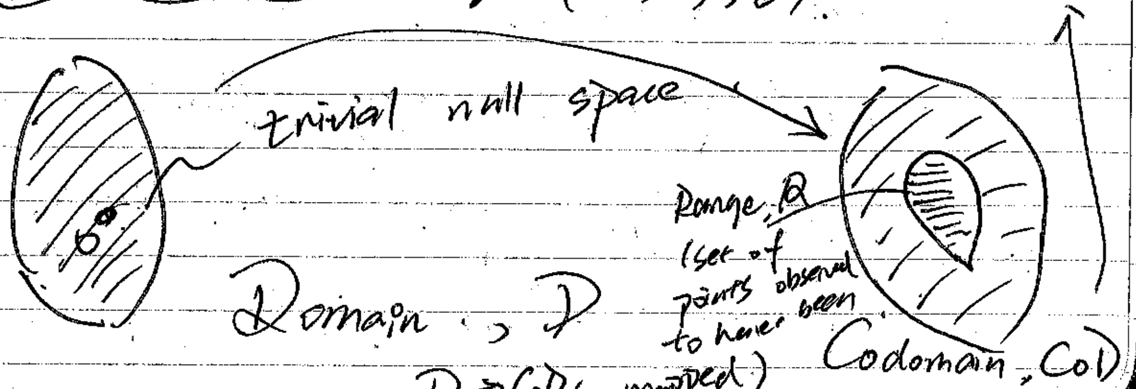
biased in its measurement.

Class 2

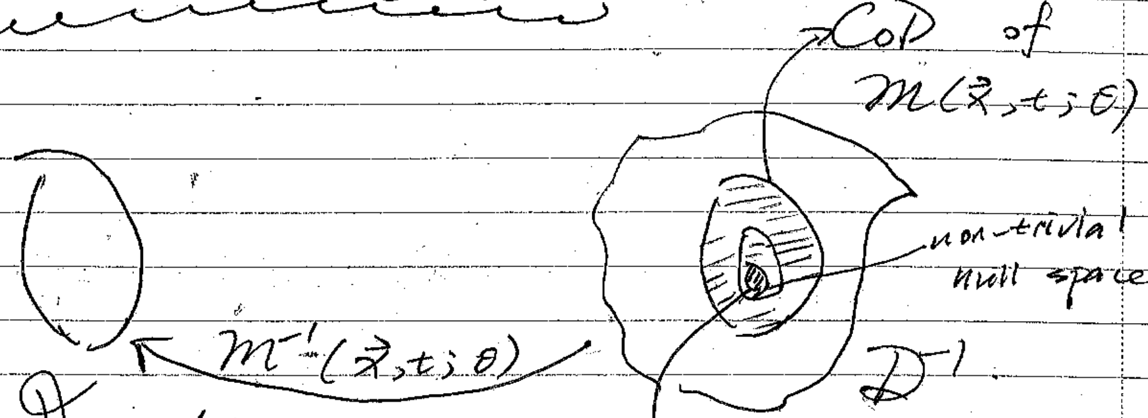
$$\text{cause}^* \rightarrow \boxed{m(\vec{x},t;\theta)} \leftrightarrow \text{effect}^*.$$

Forward Problem.

$m((\vec{x},t);\theta)$.



Inverse Problem Class 1



$\mathcal{D}$ under forward map: $\mathcal{D}_{m(\vec{x},t;\theta)}$.

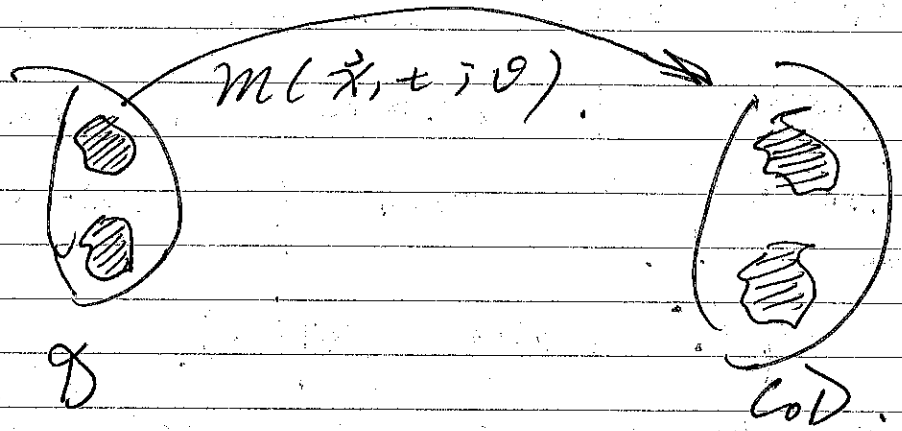
observation under $m(\vec{x},t;\theta)$

$\mathcal{R}_{m(\vec{x},t;\theta)}$.

≡ domain of inverse operator

$\vec{y} \in \mathcal{D}^{-1}$ may have no image in $\mathcal{D}$ when acted upon by $\mathcal{M}^{-1}(\vec{y},t;\theta)$, i.e. $\mathcal{M}^{-1}(\vec{y},t;\theta)$ maybe a "left inverse" of the forward $\mathcal{M}(\vec{x},t;\theta)$. Said another way $\mathcal{M}^{-1}(\vec{y},t;\theta)$ may furnish results $\vec{x} \notin \mathcal{D}$ for pre-images. $\vec{y} \in \mathcal{D}^{-1}$ $\wedge$ $\vec{y} \notin$ CoD of $\mathcal{M}(\vec{x},t;\theta)$

Inverse Problem Class 2



We will now introduce some basic concepts from functional analysis that we'll come to find are useful in our study of inverse offering important abstractions, leading to underlying theory.

elusive speaking. a generalization of concepts from finite dimensional normal vector spaces, to infinite dimensional topological spaces.

we will generalize notions of directed line segment scalars. size these and general notions of distance by capturing their essence in terms of axioms

Vector space (linear space).

let $\mathcal{X}$ be a set & $\mathbb{K}$ a "field". (e.g. $\mathbb{R}$, $\mathbb{C}$). whose elements, $\alpha, \beta \in \mathbb{K}$, we refer to as "scalars". $\mathcal{X}$ is called a "vector space" if it has an ~~operation~~ opperation called "addition", and "multiplycation" by a ~~so~~ scalar. and satisfy the following axioms.

1. $\forall.\ u, v \in \mathcal{X}$ and scalars α, β, $\alpha u + \beta v \in \mathcal{X}$.

2. $u + v = v + u$ and $u + (v + w) = (u + v) + w$

~~satisfy~~ for all: $\forall\ u, u, w \in \mathcal{X}$.

3. $\exists\ 0 \in \mathcal{X}$, called the "zero element",

there exists

such that $u + 0 = u$, $\forall u \in \mathcal{X}$.

4. $\forall u \in \mathcal{X}$, $\exists\ -u \in \mathcal{X}$. s.t.

$u + (-u) = 0$.; then by "difference" we mean $u + (-u)$ $u - v$

5. $(\alpha\beta) u = \alpha(\beta u)$,

$\forall\ \alpha, \beta \in \mathbb{K}$ & $\forall\ u \in \mathcal{X}$.

6. $(\alpha + \beta) u = \alpha u + \beta u$. & $\alpha(u + v) = \alpha u + \alpha v$.

$\forall\ \alpha, \beta \in \mathbb{K}$ & $u, v \in \mathcal{X}$.

7. $1 \cdot u = u$

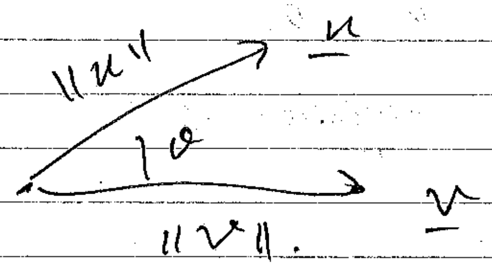
when $\mathbb{K} = \mathbb{R} \rightarrow$ real vector space

$= \mathbb{C} \rightarrow$ complex.

subspace: a subset y of a particular space x, that satisfies all axioms associated with the structure of x is called "a subspace of x"

Week 2. lecture 1.

Generalize the idea of dot product.



$\underline{v} \cdot \underline{u} = |v||u| \cos\theta.$

$v \perp u \Rightarrow u \cdot v = 0.$

$v \parallel u \Rightarrow u \cdot v = |u| \cdot |v|$

Generalize over a Complex Vector Space.

Axioms:

Let x be a complex vector space

we define an "inner product" on x.

s.t. $\langle u, v \rangle$ with $u, v \in x$, as an operation that satisfies ~~fr~~ 4 axioms.

1. $\langle u, v \rangle \in \mathbb{C}$ (summarized as "scalar" output.)

2. $\langle v, u \rangle = \langle u, v \rangle$ (conjugate symmetry)

3. $\langle \alpha u + \beta v, w \rangle = \alpha \langle v, w \rangle + \beta \langle v, w \rangle$.

4. $\langle u, u \rangle \geq 0$, and $\langle u, u \rangle = 0$,
iff $u = 0$.
(positive definiteness)

A vector space endowed w/ an inner product $(X, \langle \cdot, \cdot \rangle)$. is called an "inner product space".

e.g. consider $u(x) = \sin(x)$,
& $v(x) = \cos(x)$ ...

when $u, v \in L^2(-\pi, \pi)$. w/ u & v being real valued $\langle u, v \rangle .= \int_{-\pi}^{\pi} \sin(x) \cos(x) dx = 0$

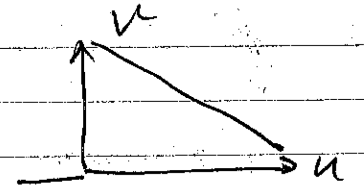
thus u & v are "orthogonal"
in $L^2(-\pi, \pi)$.

Generalizing now the notion of Scalar magnitude for our abstract vector, we the notion of a "norm".

Axioms: (axioms of norm).

for any $u, v \in X$ and $\alpha \in K$,
we define a "norm", $\| \cdot \|$, on X to be an operation satisfying:

1. $\|u\| \in R$ ("length" is real number).
2. $\|u\| \geq 0$ & $\|u\| = 0$ iff $u = 0$
(positive definiteness)
3. $\|\alpha u\| = |\alpha| \, \|u\|$. (positive homogeneity)
4. $\|u + v\| \leq \|u\| + \|v\|$.



triangle inequality.

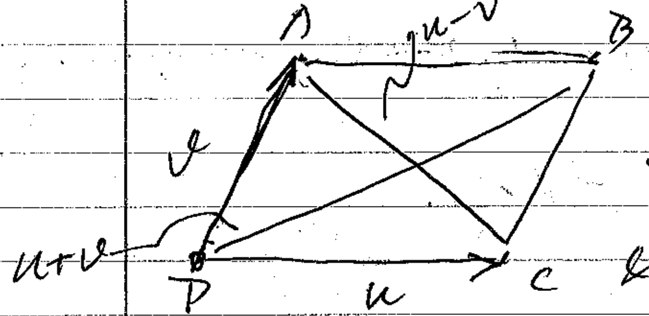
A vector space endowed with a norm, $(X, \| \cdot \|)$, is called a "normed space"

While the norm is more primitive than the inner product, the former may be generated

"L^2 norm"

from the latter. Let $u \in (X, \langle \cdot, \cdot \rangle)$. then $\|u\| = \langle u, u \rangle^{1/2}$. and we say this is a norm generated by the inner product.

While all inner products generate norms, the converse is not generally true, To see this, recall the parallelogram identity from Euclidean Geometry in 2D.
(All inner products satisfy this).



Since ABCD is a parallelogram, then $\overline{AB} = \overline{DC}$ & $\overline{DA} = \overline{CB}$.

Furthermore, $2\overline{AB}^2 + 2\overline{BC}^2 = \overline{AC}^2 + \overline{BD}^2$.
(parallelogram identity).

rewrite in terms of vectors

$$\|u+v\|^2 + \|u-v\|^2 = 2(\|u\|^2 + \|v\|^2)$$

If a norm does not satisfy this identity, then it could not have been generated from an inner product.

Given a vector space X, having two alternative norms, $\|\cdot\|_A$ & $\|\cdot\|_B$, these norms are said to be "equivalent" if there are positive constants m & M, s.t.

$$m\|u\|_A \le \|u\|_B \le M\|u\|_A$$

$\forall u \in X$, All finite dimensional norms (norms, in a finite space) are equivalent.

- Abstracting the notion of distance leads us to the axioms defining a "metric", $d(\cdot, \cdot)$.

Axioms. $\forall u, v, w \in Y$, where Y is a set (note: vector space required).

1. $d(u, v) \geq 0$, & $d(u, v) = 0$ iff $u = v$.

2. $d(u, v) = d(v, u)$.

3. $d(u, w) \leq d(u, v) + d(v, w)$

A set Y, along with a metric is termed a "metric space" & satisfies denoted as (Y, d).

While the metric is more primitive than the inner product or norm, we can generate a metric from a norm: $d(u,v) \equiv \|u - v\|$.

Our discussion of inverse problems will involve a "problem domain" where some response (effect) will be observed. Let Ω denote a simply connected, non-empty, open set in $\mathbb{R}^n$ having a Lipschitz $\partial\Omega$. $C^k(\Omega)$ denotes the space of functions, f, such that for any positive integer, k. f exists & is continuous (i.e. $f \in C^0$), and the same applies to all of f's derivatives up through order k.

A Hilbert space, $\mathcal{H}$, is a real or complex inner product space, having inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ that is also complete* metric space. w.r.t. distance function induced by the inner product.

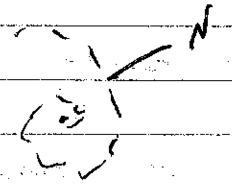
i.e. let $x, y \in$ metric space, M.

$$d(x,y) = \underbrace{\|x-y\|_{\mathcal{H}}}_{\text{inner product}} = \sqrt{\langle x-y, x-y \rangle_{\mathcal{H}}}$$

* Every Cauchy sequence of pts, in M, has a limit also in M.

$f_n, f_m \in M$. given $r > 0$, $\exists\, n, m > N$, s.t. $d(f_n, f_m) < r$

We will use the symbol $\to$ to denote strong convergence in the norm ("norm convergence") i.e. $f_n \to f$ indicates as $\lim_{n \to \infty} \|f_n - f\| = 0$, for some suitable norm.



(point-wise)

Week 2. Wed.

Let $f \in S \subset \mathcal{H}$. The "orthogonal complement" of S consists of all elements $g \in \mathcal{H}$, s.t. $\langle f, g \rangle = 0$, and is denoted by $S^{\perp}$. The "sum of two sets", $S + T$, is the set $S+T \equiv \{s+t : s \in S, t \in T\}$ & for $s \in \mathcal{H}$, $s + T$ indicates $\{s\} + T$

We will sometimes employ "little o" notation: $f(\alpha) = o(g(\alpha))$. as $\alpha \to \alpha_*$ iff $\lim_{\alpha \to \alpha_+} \frac{f(\alpha)}{g(\alpha)} = 0$.

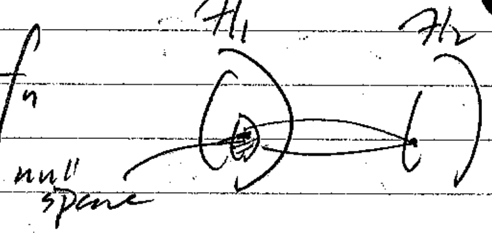
Let $A : \mathcal{H}_1 \longrightarrow \mathcal{H}_2$ be some "operator" (i.e. a map from one function space to another). The Range of A, R_A is $\{A(f) \mid f \in \mathcal{H}_1\}$.

denote Hilbert spaces; but the definition applies to arbitrary normed spaces, required for speaking about continuity:

$A: A(f_n) \to A(f_*)$ whenever : $f_n \to f_*$

inner product → natural plane to solve differential equations

usually written as Af_n



The "null space" of A, Null (A).

consists of $\{f \in \mathcal{H}_1 \mid Af = 0\}$.

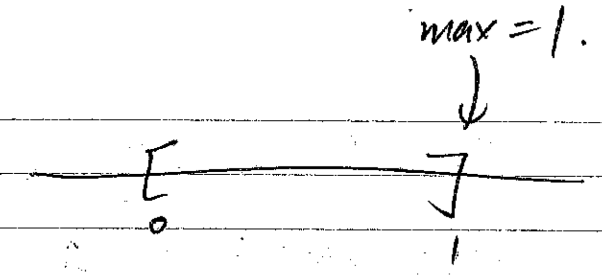
Consider a linear operator $A: \mathcal{H}_1 \to \mathcal{H}_2$

A is bounded iff the (in this case) induced operator norm is finite.

$$\|A\| \equiv \sup_{\|f\|_{\mathcal{H}_1}=1} \|Af\|$$

sup ≡ supremum least upper bound.

☆ isomorphismly
☆ inverse operator

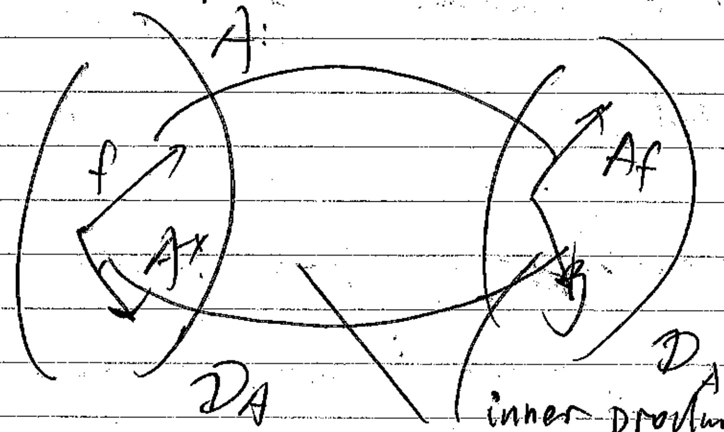


All bounded linear operators are continuous. (iff). ← both ways.

The space of bounded operators from Hilbert space $\mathcal{H}_1$ to $\mathcal{H}_2$ is denoted by $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$. The Hilbert adjoint of A is the operator $A^* \in \mathcal{L}(\mathcal{H}_2, \mathcal{H}_1)$ characterized by: $\langle Af, g \rangle_{\mathcal{H}_2}$

$$= \langle f, A^* g \rangle$$

whenever $f \in \mathcal{H}_1$, $g \in \mathcal{H}_2$



if $A = A^*$.

inner products the same.

$\underline{A}$ is self adjoint is $A = A^*$. (Then

lnfwid. s.f ~~the~~ joint $A = A^*$),

$A^{1} = \frac{-dvec(x)}{nelrapess}$ (v. ∂f $d_L = \gamma_{3}$,)

$A^{11} = \frac{adj(\underline{A})}{adj(A)}$ is nect an us

when abo bonded, sufficient l. tenor

linear corp J. if thus

$A^{\pm} = 9$

The (eigen values, given fontal).

① All eigenvalues of A, λ, (if exist) are real;

② Eigenfunctions, corresponding (necessarily) different eigenvalues are mutually orthogonal

In such cases we have:

infimum.
greatest lower bound.

$$\lambda_{min}(A) \equiv \inf_{\|f\|_{\mathcal{H}}=1} \langle Af, f \rangle_{\mathcal{H}}.$$

$$\lambda_{max}(A) \equiv \sup_{\|f\|_{\mathcal{H}}=1} \langle Af, f \rangle_{\mathcal{H}}$$

If A is "positive semidefinite" then $\lambda_{min}(A) \geq 0$. If A is positive definite, then $\langle Af, f \rangle > 0$ whenever $f \neq 0$

A is "strongly positive" if $\lambda_{min}(A) > 0$.

when A is self adjoint, $\|A\| = \max(|\lambda_{min}|, |\lambda_{max}|)$.

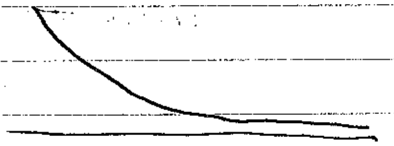
Example. $f_1, f_2, f_3, \ldots \in f$. and

$g_1 \, g_2 \, g_3 \, \dots \in g$.

and $f, g \in \ell^2(\mathbb{R})$. i.e. $\sum_{j=1}^{\infty} f_j^2 < \infty$

↳ has to "die off / converge"

which is a



Hilbert space under inner product.

$\langle f, g \rangle_{\ell^2} \equiv \sum_{j=1}^{\infty} f_j g_j$. & it possesses

an induced norm $\|f\|_{\ell^2} = \sqrt{\sum_{j=1}^{\infty} f_j^2}$.

we define the "diagonal operator" on $\mathbb{R}$

$[Df]_j = d_j f_j$.

$$\begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{bmatrix}.$$

Week 3 lecture 1

Example:

$f_1, f_2, \dots \in f$ and

$g_1, g_2, \dots \in g$. $f, g \in l^2(\mathbb{R})$

i.e., $\sum_{j=1}^{\infty} f_j^2 < \infty$. which is Hilbert s. under the inner product $\langle f, g \rangle_l \equiv \sum_{j=1}^{\infty} f_j g_j$, and it possesses an induced norm.

$$\|f\|_{l^2} = \sqrt{\sum_{j=1}^{\infty} f_j^2}$$

We define the diagonal operator on $\mathbb{R}$:

$$[Df]_j \equiv d_j f_j \quad j = 1, 2, \dots$$

$$d_j \in \mathbb{R}$$

D is bounded, iff the $B \equiv \sup |d_j| < \infty$

in which $\|D\| = B \hookleftarrow$

$\downarrow$

D is self adjoint

$\hookrightarrow \langle g, A f \rangle = \langle A^* g, f \rangle$.

D is self adjoint. $\sum_{j=1}^{\infty} d_j f_j g_j = \sum_{j=1}^{\infty} d_j g_j f$

Example.

The space of real-valued, ~~space~~ square-integrable functions on Ω, $L^2(\Omega)$, is a Hilbert space under the inner product

$$\langle f_j g_j \rangle_{L^2} = \int_\Omega f(x) g(x) dx$$

e.g. $\langle \sin(x), \cos(x) \rangle_{L^2} = \int_{-\pi}^{\pi} \sin(x) \cos(x) dx = 0$

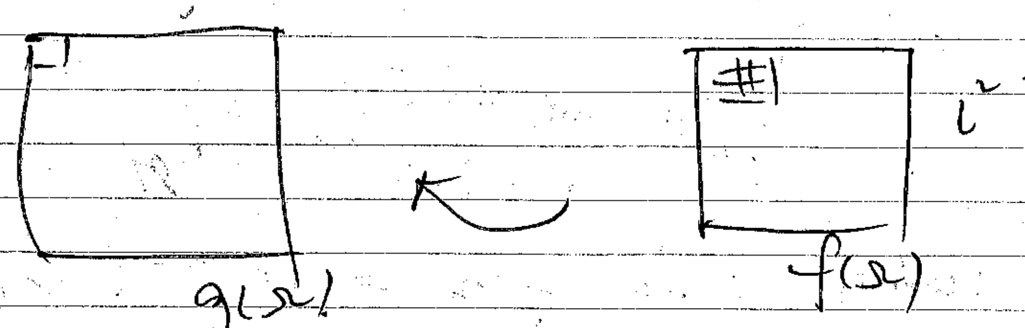
square integrable $f \in L^2(\Omega)$

$$\int_\Omega f(x)^2 dx < \infty$$

With introduce norm $\|f\|_{L^2} = \sqrt{\int_\Omega f^2(x) dx}$

The Fredholm first kind of integral operator:

$$[Kf](x) = \int_\Omega \underbrace{k(x,y)}_{\text{kernel function}} f(y) dy \quad x, y \in \Omega$$



$[kf](x)$ is bounded if $B \equiv \iint_\Omega k(x,y)^2 dx dy < \infty$,

in which case $\|[kf]\| = \|k\| \le \sqrt{B}$.

The adjoint of k is given by

$$[k^* g](y) = \int_\Omega k(y,x) g(x) dx, \quad x, y \in \Omega$$

and k is self-adjoint iff the kernel function is symmetrical: $k(x,y) = k(y,x)$

<u>"Best Approximation" within a Hilbert space</u>

↳ a core in FEA.

Let $f \in H$ & $g \subset H$, $s^* \in S$ is called the best approx. to f, within

S, if:

$$S_* = \underset{s \in S}{\operatorname{argmin}} \underbrace{\| s - f \|_{\mathcal{H}}}_{\text{induced norm}}$$

meaning $\| S_* - f \|_{\mathcal{H}} \leq \| s - f \|_{\mathcal{H}} \ \forall s \in S$

provided ~~that~~ S is closed with $\mathcal{H}$. ~~then~~ S_* exists. If it exist, is unique. Such as the case when S is a finite dimensional subspace of $\mathcal{H}$.

Theorem : Best approximation on Hilbert space.

If S_* is the best approximation to f ~~∈a~~ $\in \mathcal{H}$, within $S \subset \mathcal{H}$, then

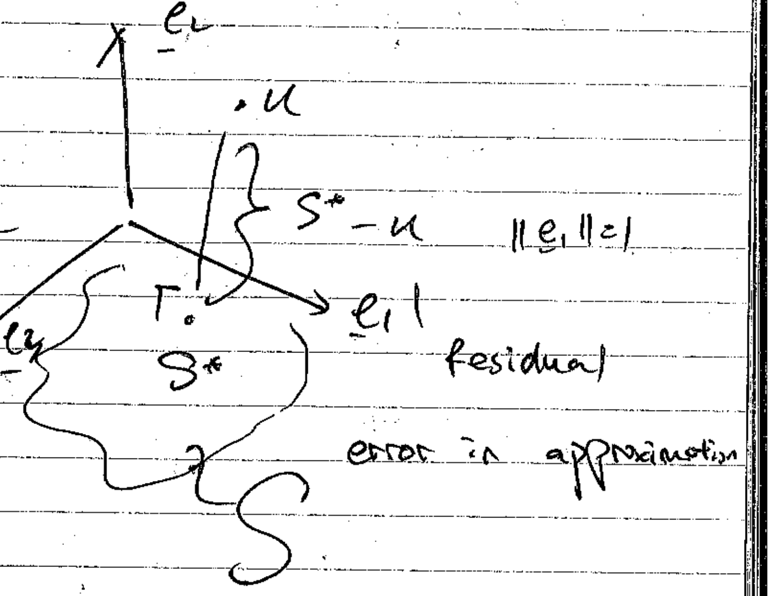
$$< S_* - f, s >_{\mathcal{H}} = 0$$

whenever $s \in S$.

Example PDE. $\frac{\partial^2 u(x, y, z)}{\partial x^2} + \frac{\partial^2 u(x, y, z)}{\partial y^2} + \frac{\partial^2 u(x,y,z)}{\partial z^2} = f(x, y, z)$

Soln $u(x, y, z)$

Given this Theorem, along with a finite dimensional orthonormal basis for subspace S,



$\{\phi_1, \phi_2, \dots, \phi_n\}$, the formula for computing the best approximation within S_*

~~$\#$~~ $S_* = \sum_{i=1}^{n} \alpha_i \phi_i$, $\alpha_i \in \mathbb{R}$ & $\phi_i \in S$.

having representation

$$S_* = \sum_{i=1}^{n} \underbrace{< f, \phi_i >}_{\text{projection of } f \text{ onto } \phi_i} \phi_i$$

Week 3. Thurs.

Well-posed problem.

Consider $K : \mathcal{H}_1 \to \mathcal{H}_2$.

$$\text{s.t. } Kf = g$$

$$\forall f \in \Omega \subset \mathcal{H}_1$$

$$g \in \mathcal{H}_2.$$

and let it be well-posed in the sense of Hadamard. In such a case, K has a well-defined, continuous inverse. $K^{-1}(Kf) = f$. for any $f \in \Omega$ &

$$R_K = \mathcal{H}_2.$$
$$\Updownarrow$$
$$\text{COD}_K = \mathcal{H}_2.$$

* { Recalling Hadamard's requirement for well posedness:

① Existence

② uniqueness <=> trivial null space.

③ Stability. => For inverse solution to be stable:

if $Kf_* = g_*$ & $Kf = g$; then $f \to f_*$ whenever $g \to g_*$.

$$\begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{bmatrix} \begin{Bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{Bmatrix} = \begin{Bmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{Bmatrix}. \qquad \text{or } l^2(\mathbb{R})$$

$\uparrow$

Consider again, our diagonal operator, D, but now with $d_j = 1/j$, $j = 1, 2, \cdots \infty$.

If a solution to $Df = g$ exists, then its unique since D is linear. & $\text{Null}(D) = \{0\}$.

Now, perhaps we are given an effect, $g = (1, \frac{1}{2}, \frac{1}{3}, \ldots)$ that lives in $l^2(\mathbb{R})$ and asked to determine the cause: find f.

because $g \notin R_D$. because the only element able to produce g is $f = (1, 1, \ldots)$.
$\notin l^2(\mathbb{R})$

Thus we see D is still ill-posed within the context of inverting from g

Stability is also lacking in this operator, D, to see this, take $f_n \in \ell^2(\mathbb{R})$ to be the δ_{nj}, for its j^{th} components

$$\delta_{nj} = \begin{cases} 1, & n=j \\ 0, & \text{else} \end{cases}$$

i.e. $f_1 = (1, 0, 0, \ldots)$ & $f_2 = (0, 1, 0 \ldots)$ ...

As we proceed with more f_ns, we observe that $\|Df_n\| = \frac{1}{n} \to 0$, but $\|f_n\|_{\ell^2}$ is always 1. Condition 3 is not always satisfied.

We can remedy this instability by adjusting our norm, Let $D : \mathcal{H}_1 \to \mathcal{H}_2$, $\mathcal{H}_1 = \ell^2(\mathbb{R})$ but now let $\mathcal{H}_2$ be the space of infinite sequences, g, that satisfy

$$\|g\|^2_{\mathcal{H}_2} \doteq \underbrace{\sum_{j=1}^{\infty} j^2 g_j^2}_{\text{satisfies axioms of Norm}} < \infty$$

Since $g = Df$, applying our new norm yields

$$\|g\|^2_{\mathcal{H}_2} = \sum_{j=1}^{\infty} j^2 (Df)^2 = \sum_{j=1}^{\infty} j^2 \frac{1}{j^2} f_j^2$$

$$= \sum_{j=1}^{\infty} f_j^2$$

$$= \|f\|^2_{\ell^2}.$$

thus, $\|Df\|_{\mathcal{H}_2} = \|f\|_{\mathcal{H}_1}$, & $Df = g$, is now well-posed.

In practice, one is usually unable to "define away" ill-posedness by arbitrarily changing topologies, as the problem itself may dictate that a specific Topology is req'd to make phys. sense

- Compact Operators. (Bounded, linear, operators, that admit a generalization of the spectral theory) $\rightarrow A = \Psi^{*} \Lambda \Psi$.

Compact operators frequently occur within problem settings ~~that~~ are ill-posed.

A bounded linear operator, $K: \mathcal{H}_1 \to \mathcal{H}_2$ is compact iff the image of a bounded set under the action of K, becomes a relatively compact set: meaning the closure of this image is a compact subset of $\mathcal{H}_2$.

Examples of the compact operators are the "diagonal operator" from our earlier example. Fredholm 1st kind integral Eqn, as well as any linear operator having a finite dimensional Range. (e.g. ~~anything~~ matrix operator)

__Thm__: (Ill-posedness of a compact operator) Let $K: \mathcal{H}_1 \to \mathcal{H}_2$ be a compact linear operator & let $\mathcal{H}_1$ & $\mathcal{H}_2$ be infinite dimensional. If the range of K is infinite dimensional, then the operator equation, $Kf = g$ is ill-posed*. (In the sense that Hadamard's 1st & 3rd conds are violated). If the range of K has finite dimension, then $Kf = g$ is also ill-posed**. (Hadamard's second condition violated).

* In this case, $\overset{\text{range of } k}{R_k}$ is not closed. (close iff $\dim(k) < \infty$)

** Since $\mathcal{H}_2$ is infinite dimensional, a finite range $R_k \Rightarrow \dim(\text{Null}(k)) = \infty$. Having other than a trivial null space destroys uniqueness in the inverse sol'n to $K.f = g$.

If K is compact, then the operator

K^*K is also compact, & self-adjoint.

adjoint From the spectral theory of compact, self-adjoint operators, [Kreyszig. Intro. Functional Analysis with Apps., Chap. 9], there exist positive eigenvalues, λ, (at most countably infinite numbers, in which case their point of accumulation is zero), along with a corresponding set of orthonormal eigenfunctions, λ that forms a basis for $Null(K^*K)^\perp = Null(K)^\perp$

From this, we can construct "a singular system" from this eigendecompositions.

$$\left(\lambda = \nu_j,\ s = \sqrt{\lambda_j},\ u_j = \frac{K\nu_j}{s_j}\right)$$

Week 4. Lecture 1

Compact Linear Operator:

$K: \mathcal{H}_1 \to \mathcal{H}_2$, its "singular system" comprises a countable set of triples, $\{u_j, \mu_j, \nu_j\}$ possessing the following properties:

1). $\overset{\text{span}}{Sp}(\nu_i) = Null(K)^\perp$

2). $Sp(u_j) = \bar{R}_K$

3). $\mu_1 \geq \mu_2 \dots \geq \mu_j > 0$

$\nu_j \mid u_j$ each comprise an orthonormal sets.

Furthermore, if $\dim(R_K) = \infty$

$$\lim_{j \to \infty} \mu_j = 0$$

As noted previously, the First kind Fredholm Integral operator, $[Kf](x) = \int_\Omega d(x, y) f(y) dy = g(x)$

Is a compact operator → in inverse prob.

These would be thought of as the generalization.

of the finite rank / finite dimensional, linear

algebraic context $[A]\{f\}=\{g\}$ to the

in infinite rank / infinite dimensional

setting in ~~ketz~~ Hilbert space

Fredholm Integral of 1st kind.

General ~~Form~~:

$$\int_0^1 \underbrace{k(s,t)}_{\text{kernel}} f(t)\,dt = g(s) \quad 0\le s\le 1$$

compact operator / strictly continuous

under the

$m=(s,\theta)$ Banach space

and $\mathcal{M}(\Sigma; m)$: $f(x-t) - g(s)$

$[kf]\neq$

When $m(s;\theta)$ has a fin dimensional

null space & coarse range. with $k(s,t)$

$[kf(\theta)] = g(s)$

An important special case occurs when $k(s,t)$

is som translational invariant func.

i.e. $k(s,t) := h(s-t)$ → Class 2 inverse

prob, with this type of kernel func,

Constitutes the classical "deconv."

problem (conv. Thm. $\mathcal{F}(h(-t)) = H \cdot \mathcal{F}(f(-t))$

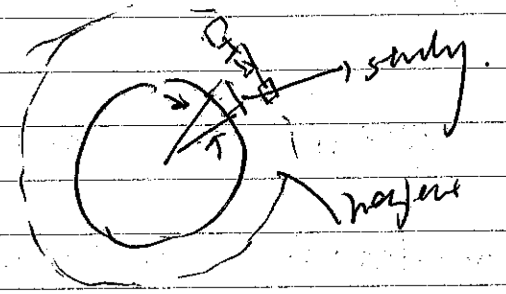
$= F \rightarrow H \times F = G$.

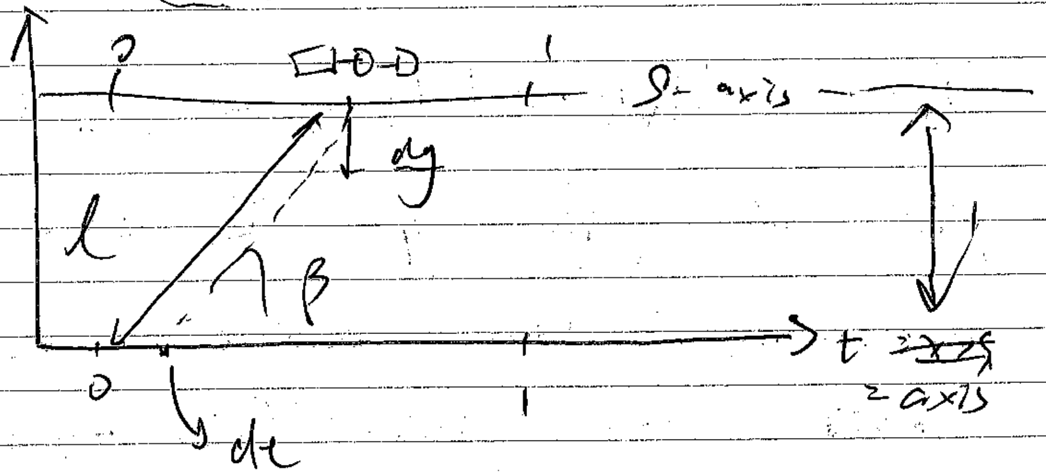
e.g. for 1D case.

$$\int_0^1 k(s-t) f(t)\,dt = g(s) \quad 0\le s\le 1$$

This form arises in a fun example: Gravity

Surveying problem. Consider a problem where some mass distribution, f(t), is positioned at some depth, d, below the orbital path of some spacecraft.





$f(t) \equiv$ 1 D mass density

We are able to measure the gravitational pull downward: g, given g(s) find f(t).

~~Universing~~ Newton Law.

$$\text{Force} = G\frac{\text{Force}_1\,\text{Force}_2}{\cancel{\text{Area}}\ r^2}$$

$f(t)\cdot dt \Rightarrow$ mass @ H7.

If we hold this "Source Pt.", t, fixed, we may use Newton's law to compute gravitational attraction at each of the "field points", s, as:

$$dg = \frac{\sin\beta}{r^2} f(t)\,dt. \quad r = \sqrt{d^2+(s-t)^2}$$

recognizing that $\sin\beta = \frac{d}{r}$, we obtain

$$dg = \frac{d}{(d^2+(s-t)^2)^{3/2}} f(t)\,dt.$$

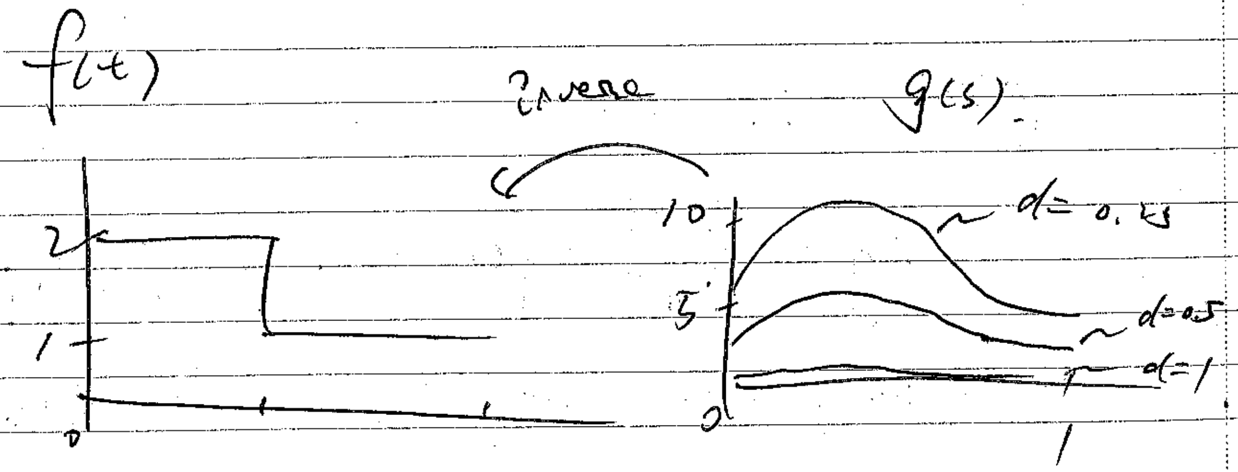
Thus, the total value of g(s) for $0 \le s < 1$.

Includes the contributions from all the mass along the t-axis. g

$$g(s) = \int_0^1 \underbrace{\frac{d}{(d^2+(s-t)^2)^{3/2}}}_{\text{kernel function}} f(t)\,dt.$$

~ function of s.

conceptual forward problem results.



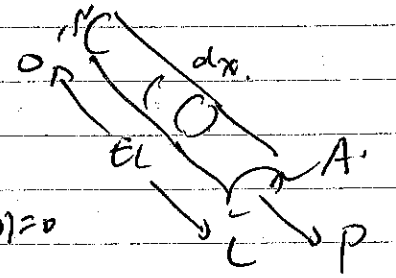
* the precise reason ~~that~~ supports this smoothing behavior may be found from a specialization of the Riemann-Lebesgue Lemma. where we decompose our mass distribution function into harmonics, as (Fourier basis

$$f_p(t) = e^{-ipt}, \; p = 1, 2, \ldots$$

(ignore scaling)

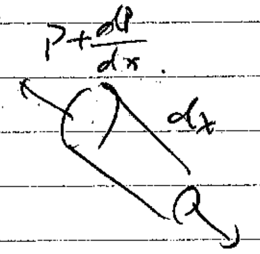
Week 4. lecture 2.

HW.



B.C.s. $u(0)=0$

FBD



$P = \sigma A = E\varepsilon A$

Engineering strain $\frac{\Delta L}{L}$ ↑

From Newton's 3rd law.

Forward model.

$\sum f_x = 0 \rightarrow \frac{dP}{dx} = 0$

$P \rightarrow$ constant.

$\mathcal{M}(u(x), AEP)$

cause → effect.

$P \rightarrow u.$

$\int \frac{P}{EA} dx = u.$

$\downarrow \quad EA\frac{du}{dx}$

Inverse problem

$\frac{Px}{AE} + C = u(x)$

$\mathcal{M}(P, AE\ u(x)) \quad P \leftarrow u.$

$EA\frac{du}{dx} \leftarrow$ possedness.

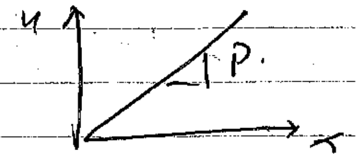
Ideal inverse problem is well-posed.

Existence: $P \in C(0,L)$.

$u \in C(0,L) \quad u(0) = 0.$

Uniqueness: Since EA = const.

P is const. then



Stability when EA = const. &

$u \in C(0,L)$

$P \in C(0,L)$.

$\varepsilon\delta$. const

satisfied → continuity in seq.

Noisy case

$P_{est} = EA\frac{du_x}{dx}[1 + \varepsilon \sin(\omega x)] + EAu_A\omega$

$\varepsilon \cos(\omega x)$.

messes with stability.

$A_r\{d\}A_\omega = \{g\}$

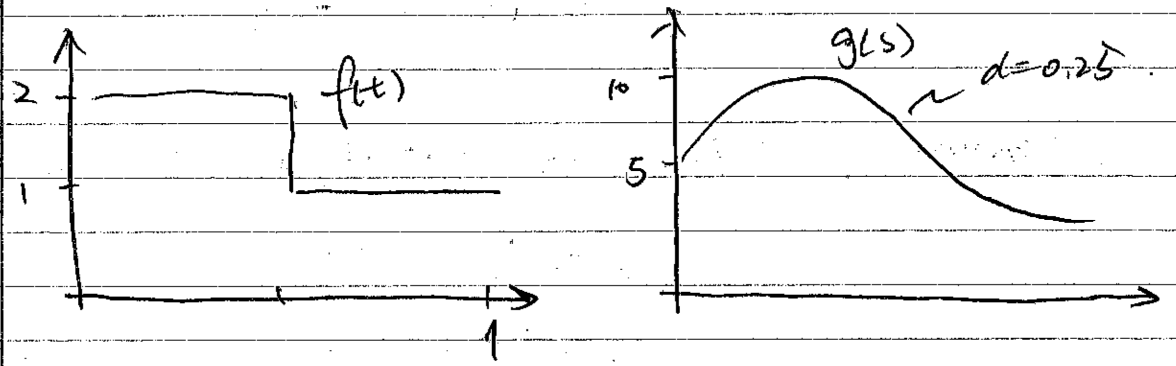
$[k]\{f\} = \{g\}$ Violates Uniqueness.

$\underline{A} = \underline{A_r}\,\underline{A_c}$

$\{f\} \overset{!!}{=} [k]^{-1}\{g\}$

Gravity Survey. ex.

$$g(s) = \int_0^1 \frac{d}{(d^2+(s-t)^2)^{3/2}} f(t)\, dt.$$



we can understand this smoothing behavior in light of the Riemann-Lebesgue Lemma.

Let's imagine decompose our mass distribution $f(t)$ into Fourier modes

$$f_p(t) = e^{-ipt}, \quad p = 1, 2, \ldots$$

$K(s,t)$ with constant "s" is an element (ignore scaling) L_2, or L^2, $\Rightarrow L^2 \subset L^1$

↑ req'd for R-L Lemma.

R-L Lemma states.

$$g_p(s) = \int_0^1 k(s,t)\, f_p(t)\, dt \to 0$$

as $p \to \infty$

As a result of R-L lemma, we sense a problem brewing for our deconvolution inverse problem: if we are to recover $f(t)$ from smooth $g(s)$, then we must amplify the small (high frequency) harmonics.* of the latter

* Think Fourier series of our step function.

to obtain the former. This is a big problems for computers (finite floating pt. precision) which would need/require infinite precision to do this.

However, In real world settings, measurement noise (unwanted signal) are ubiquitous, and ready to be amplified too

Details regarding all this will come into focus when we discuss ~~SVD~~ SVE of infinite dimensional Fredholm Int. ops. & later when discussing the discrete analogue, the "SVD"

The Integral operator of a 1st kind Fredholm integral equations is a type of "Hilbert-Shmidt" operator when it satisfies:

(H.S)
$$\int_0^1\int_0^1 k(s,t)^2\, ds\, dt < \infty$$

and in this case we say the $k(s,t)$ is "square integrable".

Any such H-S operator admits a SVE of the form

singular values.

right singular function

$$K(s,t) = \sum_{i=1}^{\infty} \mu_i\, u_i(s) v_i(t).$$

left singular function.

Integral op : $[k\cdot](s)$

$$\langle u_i, u_j\rangle = \int_\Omega u_i u_j\, ds = \delta_{ij}.$$

these function sets, each comprise orthonormal sets under L^2 inner product

$$\langle v_i, v_j\rangle = \delta_{ij}$$

and the "singular values", μ_i, form a non-increasing segeunce

non-degenerate

$$\mu_1 \geq \mu_2 \geq \mu_3 \geq \dots \geq 0.$$

If the cardinality of the non-zero singular values is finite, then we refer to the operators as being "degenerate".

$\Rightarrow$ dimension $(\mathrm{Null}(K)) = \infty$

Week 3. Lecture 1.

1st Kind Fredholm Int. Eqn. generates a H-S operator when it satisfies.

$$\iint_0^1 k(s,t)^2 \, ds \, dt < \infty$$

$$k(s,t) \in L^2(0,1).$$

"square integrable".

$k(s,t)$ is called kernel.

This H-S operator admits a spectral decomposition called "Singular Value Expansion" (SVE).

~~right~~ left singular function

$$\left.\begin{array}{l} k(s,t). \\ [K\cdot](s) \end{array}\right\} = \sum_{i=1}^{\infty} \mu_i \, u_i(s) \, v_i(t).$$

singular values.

~~left~~ singular function
right

"Hilbert - Schmidt" operator

$$\langle u_i, u_j \rangle = \int_\Omega u_i u_j \, ds = \delta_{ij} \begin{cases} 1 & j = 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\langle v_i, v_j \rangle = \delta_{ij}$$

non-generate probs.

$$\mu_1 \geq \mu_2 \geq \cdots > 0.$$

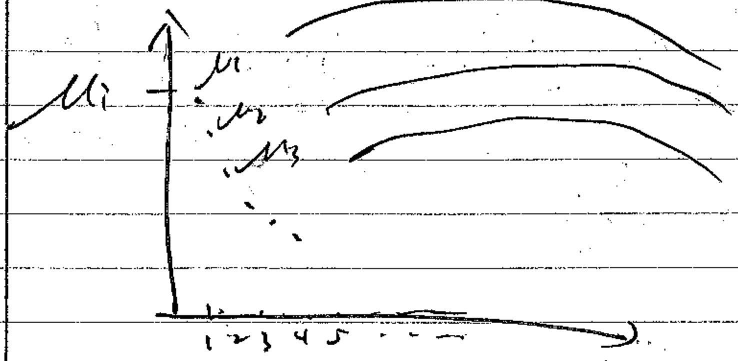
The SVE satisfies the "fundamental relation".

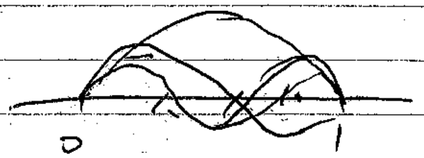
$$(\#) \quad \int_0^1 k(s,t) \, v_i(t) \, dt = \mu_i \, u_i(s)$$

$$[K]\{f\} = \{y\}.$$

$$[K]\{\cancel{x}\} = \lambda\{x\}.$$

The singular functions resemble a spectral basis in that both are orthonormal & both have increasing numbers of zero crossings as the magnitude of their singular values, or eigenvalues, respectively get small magnitude





Class I inverse probem

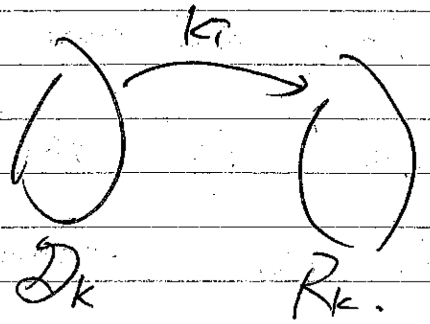
Cause $\rightleftarrows$ M $\rightleftarrows$ effect.

General form for class 1 inv. prob.

$$\int_0^1 k(s,t)\, f(t)\, dt = g(s) \qquad (*)$$

clean image

$0 \leq s \leq 1$



where $f, g \in L^2(0,1)$, we may expand these functions $f(t) = \langle v_i, f \rangle v_i(t)$

$g(s) = \langle u_i, g \rangle u_i(s)$.

span D_K (**) span R_K

subst. (**) into (*) we see:

$$\sum_{i=1}^{\infty} \langle v_i, f \rangle \int_0^1 k(s,t)\, v_i(t)\, dt$$

$$= \sum_{i=1}^{\infty} \langle u_i, g \rangle u_i(s) \qquad (\dagger)$$

Which indicates that since $V_i(t)$ resembles a spectral basis, R-L lemma ensures smoothing of $\phi g(s)$.

Additionally, from the ordering of our singular values, combined w/ our fundamental relation (#), we notice that v_i are mapped to $\mu_i u_i$. Thus offering additional insights into "damping out" of high frequencies.

(i.e. Our H-S 1st kind Fred. Integral operator is a kind "mollifier")

We can now re-express (+) more explicitly in terms of our fundamental Rel (#) to yield:

$$\sum_{i=1}^{\infty} \langle v_i, f \rangle \int_0^1 k(s,t)\, v_i(t)\, dt$$

(‡)
$$= \sum_{i=1}^{\infty} \mu_i \langle v_i, f \rangle u_i(s)$$

$$= \sum_{i=1}^{\infty} \langle u_i, g \rangle u_i(s).$$

From (‡) we notice that if our kernel is degenerate ($\mu_1 \geq \mu_2 \geq \dots \geq 0$), then we may only hold to find inv. sol'n for $f(t)$ if we knew $g(s)$. This are meaningful, when the corresponding components $\langle u_i, g \rangle u_i(s)$ are also zero. Seldom occurs in practice due to unavoidable noise. To avoid this, we consider non-degenerate case.

$$\mu_1 \geq \mu_2 \geq \dots \geq 0.$$

However, even in the non-degenerate case, there is a condition that must be met when pursuing an Inv. Sol'n.

Observe from (‡) that we have

$$\sum_{i=1}^{\infty} \mu_i \langle v_i, f \rangle u_i(s) = \sum_{i=1}^{\infty} \langle u_i, g \rangle u_i(s)$$

and so, the coeffs.

$$\langle v_i, f\rangle = \frac{\langle u_i, g\rangle}{\mu_i}$$

which when substituting into (**)

yield an expression for our Inv. Sol'n.

$$f(t) = \sum_{i=1}^{\infty} \frac{\langle u_i, g\rangle}{\mu_i} v_i(t).$$

Restrict $f(t) \in L^2(0,1)$. i.e. bounded in the induced 2-norm, $\|\cdot\|$

This leads to to "Picard Condition".

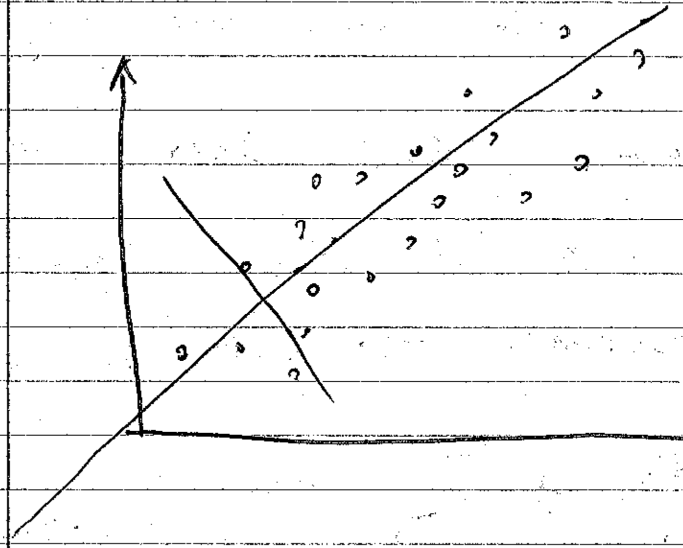
Req'd for the sol'n to our inv problem.

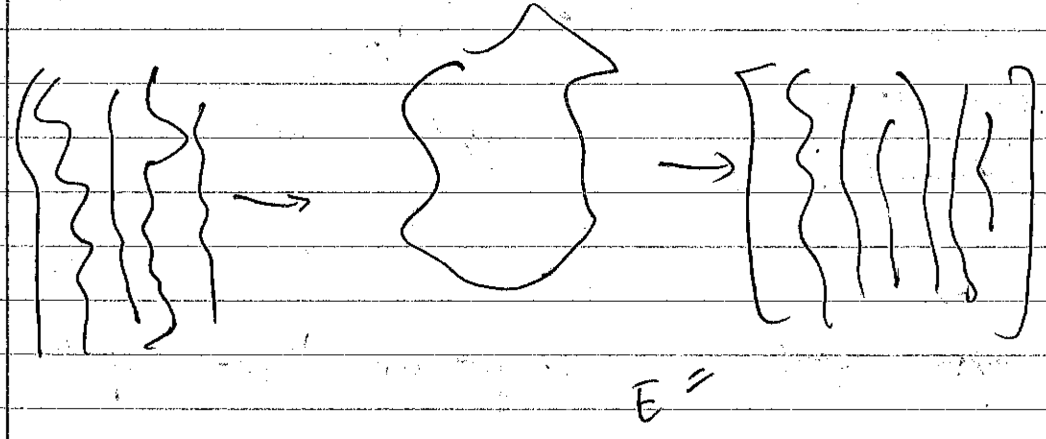
$$\|f\| = \int_0^1 f(t)^2 \, dt = \sum_{i=1}^{\infty} \langle v_i, f\rangle^2$$

$$= \sum_{i=1}^{\infty} \left(\frac{\langle u_i \; g\rangle}{\mu_i}\right)^2 < \infty$$

RHS: coeff, $\langle u_i g\rangle$. must decay more

quickly than the singular ~~function~~ values, μ_i, do.





$$U\Sigma V^T = SVD(E)$$

$\hookrightarrow U = \lambda$

$$\lambda^T \lambda \lambda = Eig(cov(E))$$

$\langle v_i, f\rangle v_i(t)$

Week 5 lecture 2.

last time: fundamental relation & the projection of the inv. sol'n $f(x)$ & observed function $g(s)$ onto the span of the right & left singular functions respectively to get an expression for inverse sol'n

$$\underbrace{f(t)}_{\text{needs to be bounded}} = \sum_{i=1}^{\infty} \frac{\overset{\text{mode}}{\langle u_i, \overset{\text{image}}{g}\rangle}}{\underbrace{\mu_i}_{\text{singular val.}}} \underbrace{v_i(t)}_{\text{right singular function}}.$$

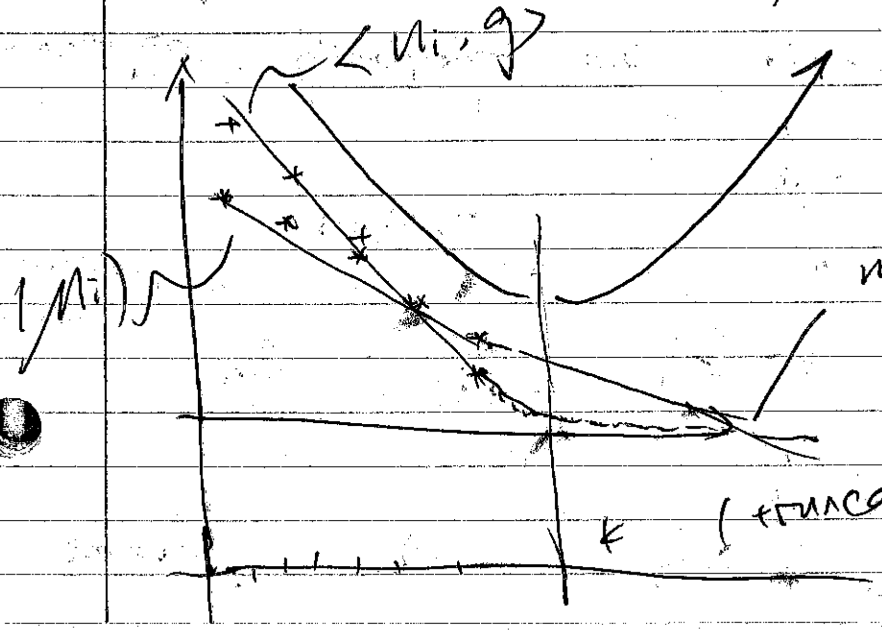
↓

we impose that (to prevent "blow-up").

$$\|f\|_{L^2}^2 = \int_0^1 f(t)^2 \, dt = \sum_{i=1}^{\infty} \langle v_i, f\rangle^2 = \sum_{i=1}^{\infty} \Big(\frac{\overbrace{\langle u_i, g\rangle}^{\text{measure}}}{\mu_i}\Big)^2 < \infty$$

⇒ RHS coeffs must "decay" more quickly than the singular vals for a meaningful sol'n to exists.

The problem with all in practice, there is always unavoidable noise contamination. In any measurement of $g(s)$, & so eventually, the coefficient, $\langle u_i, g\rangle$, will "level off" at some "noise floor", thus violating the Picard Condition ... leading to a divergent inv. sol'n, as more components are included in the expansion.



let us discretize

- Quadrature (Nyströ) methods.

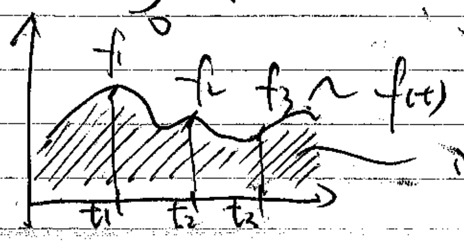
"Numerical Integration".

Let some integrable function, $f(t)$, be evaluated at special preselected pt.s, t_j, $j=1,2,\ldots,n$, such that $f_j = f(t_j)$

we may employ the approx. quadrature (numerical integration) for the discretization, t_j. to evaluate the integral of $f(t)$, sometimes exactly, but frequently, approximately)

thus we write

$$\int_0^1 f(t)\,dt = \sum_{j=1}^{n} \overset{\text{"weights"}}{W_j}\, f_j + \overset{\text{quadrature error}}{E_n}$$



integral of $f(t)$ = $\int_0^1 f(t)\,dt$.

$$w_1 f_1 + w_2 f_2 + w_3 f_3 + \Sigma$$

In the case of a Class 1 inverse prob. we can sample our known function at m locations. & enforce these on the RHS as "collocation Conditions."

$$\int_0^1 k(s,t) f(t)\,dt = \sum_{j=1}^{n} W_j\, k(s,t_j) f_j + E_n(s_i)$$

$$= g(s_i), \quad i=1,2,\ldots, m.$$

neglecting quadrature error. (usually unknown), we end up with

$$\sum_{j=1}^{n} W_j\, k(s_i, t_j) f_j = g(s_i)$$

$$i=1,2,\ldots,m.$$

It's fine for $m > n$, just solve the problem in a least square sense:

$\underset{x}{\text{argmax}} \|Ax - b\|_2$, $A \in \mathbb{R}^{n\times n}$

$x \in \mathbb{R}^n$.

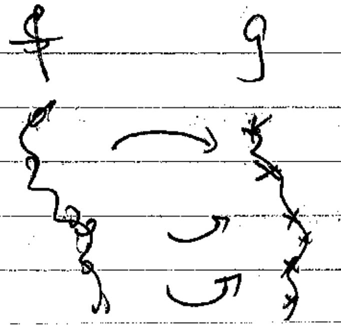
$[A]\{x\} = \{b\}$. $b \in \mathbb{R}^m$

go ahead & let $m=n$

$$\begin{bmatrix} W_1 k(s_1,t_1) & W_2 k(s_1,t_2) & \cdots & W_n k(s_1,t_n) \\ W_1 k(s_2,t_1) & W_2 k(s_2,t_2) & \cdots & W_n k(s_2,t_n) \\ \vdots & \vdots & \ddots & \vdots \\ W_1 k(s_n,t_1) & W_2 k(s_n,t_2) & \cdots & W_n k(s_n,t_n) \end{bmatrix}$$

$$\begin{Bmatrix} \bar{f}_1 \\ \bar{f}_2 \\ \vdots \\ \bar{f}_n \end{Bmatrix} = \begin{Bmatrix} g(s_1) \\ g(s_2) \\ \vdots \\ g(s_n) \end{Bmatrix}.$$

$$\underbrace{g(s_i)}_{} \approx \int k(s,t) f(t)\, dt \,.$$



more generically, as $Ax=b$, where

$$\text{Given} \begin{cases} a_{ij} = w_j k(s_i, t_j). \\ x_j = \bar{f}_j \leftarrow \text{find} \\ b_i = g(s_i). \end{cases}$$

Lec. 7 — Feb. break.

Week 6 Lecture 2

SVE ↦ SVD.

Expansion Methods

Consider two sets of mutually orthonormal functions, from two different infinite dimensional Hilbert spaces:

$$\phi_1, \phi_2, \ldots, \phi_n \in \mathcal{H}_1 \sim \text{inverse soln } f(t).$$

$$\psi_1, \psi_2, \ldots, \psi_n \in \mathcal{H}_2 \sim \text{RHS, } g(s) \text{ lives here.}$$

Petrov-Galerkin method

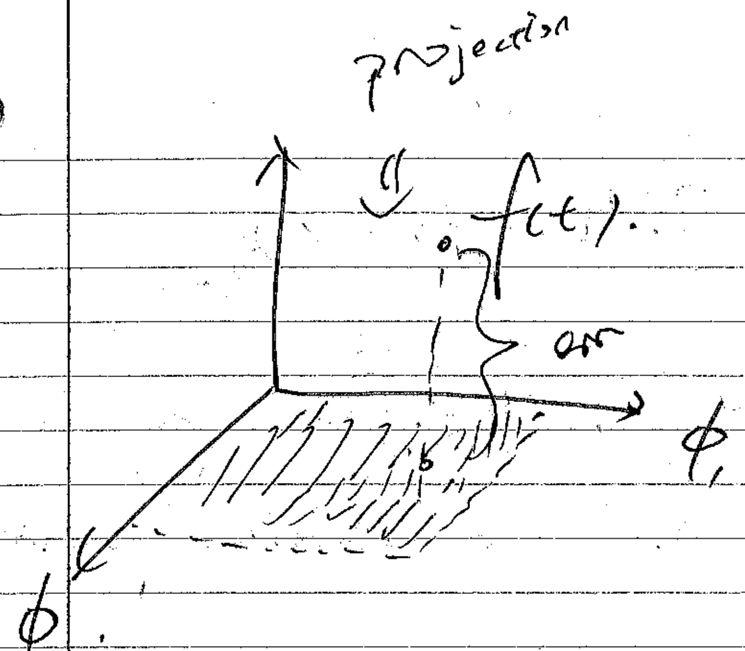
$$f(t) = f^{(n)}(t) + E_f(t);\quad f^{(n)} \in \underbrace{\text{span}(\phi_1, \ldots \phi_n)}_{\text{Selected to respect prior knowledge on inverse solution}} \subset \mathcal{H}_1$$

$$g(s) = \underbrace{g^{(n)}(s)}_{\text{Projections into respective Hilbert spaces.}} + \underbrace{E_g(s)}_{\text{Expansion errors}};\quad g^{(n)} \in \text{span}(\psi_1, \ldots \psi_n) \subset \mathcal{H}_2$$

↳ orthogonal compliment

(respect information prior know RHS)

projection



e.g.

$$f^{(n)}(t) = \sum_{j=1}^{n} c_j \phi_j(t) \leftarrow \text{Inverse soln find this!}$$

We can substitute this expansion for f(t) into our Class 1 Fredholm eqn.

$$G(s) = \int_0^1 K(s,t) \cdot f^{(n)}(t)\, dt = \sum_{j=1}^{n} c_j \int_0^1 K(s,t)\, \phi(t)\, dt.$$

As it stands, function G(s) is not our RHS, but we can project it into span$(\psi_1, \psi_2, \ldots \psi_n)$.

Giving: $G(s) = G^{(n)}(s) + E_G(t)$

$G^{(n)} \in \text{span}(\psi_1, \psi_2 \dots \psi_n) \subset \mathcal{H}_2.$

but we want $G(s) = g(s)$ so we enforce this as a collocation function.

$$G^{(n)}(s) = g^{(n)}(s)$$

$$G(s) - E_G(s) = g(s) - E_g(s)$$

$$\underbrace{G(s) - g(s)}_{\text{Residual}} = E_G(s) - E_g(s)$$

$$\Downarrow$$

Residual is orthogonal to the basis to each basis vector that spans each basis vector ψ_j.

This orthogonality in the residual w.r.t. $\text{span}(\psi_1, \psi_2, \dots, \psi_n)$ will ultimately allow us to uniquely identify our unknown inverse solution coefficients, χ_j, from:

$$\langle \psi_i, G(s) - g(s) \rangle_{\mathcal{H}_2} = 0 \; ; \; i = 1, 2, \dots, n$$

from linearity in $\langle \cdot, \cdot \rangle$, over the reals (Both slots).

$$\langle \psi_i, g(s) \rangle_{\mathcal{H}_2} = \langle \psi_i, G(s) \rangle_{\mathcal{H}_2}$$

$$= \langle \psi_i, \int_0^1 k(s,t) f^{(n)}(t)\, dt \rangle_{\mathcal{H}_2}$$

$b = Ax$

$$\langle \psi_i, g(s) \rangle_{\mathcal{H}_2} = \sum_{j=1}^{n} \chi_j \langle \psi_i, \int_0^1 k(s,t) \varphi_j(t)\, dt \rangle_{\mathcal{H}_2}$$

$$b = Ax \qquad x_i = \phi_i$$

$$b_i = \int_0^1 \psi_i(s) g(s)\, ds \qquad A_{ij} = \int_0^1\int_0^1 \psi_i(s)\, k(s,t)\, \phi_j(t)\, ds\, dt$$

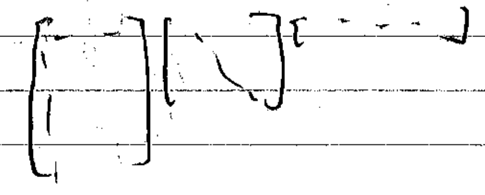
$$\langle a, b \rangle_{\mathcal{H}_2} = \int ab\, ds$$

Based on to need for more work, as compared with the quadrature method, you might be asking why would I over use the "expansion method?".

The answer to this is that ~~when~~ when we construct the Matrix SVD, of the discrete problem, then we have a well understood relation between the SVD of the discrete problem & SVE in the continuum problem thus enabling the specification of the "Discrete Picard Cond.".

We now introduce the SVD for any matrix, $A \in \mathbb{R}^{m\times n}$, with $m \geq n$:

$$A = U\Sigma V^T = \sum_{i=1}^{n} u_i \sigma_i v_i^T$$



where U is $m\times m$ unitary matrix

orthogonal if real matrix

$U^T = U^{-1}$

$U^* = U^{-1}$

Hermitian transpose

conjugate transpose.

Σ is an $m\times n$ rectangular, diagonal matrix & V is an $n\times n$ unitary matrix, with $\Sigma = \text{diagonal}(\sigma_1, \sigma_2, \dots, \sigma_n, 0, \dots 0)$, with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$.

in SVE, these were μ_i

$U^TU=I \quad V^TV=I$

and the inverse of A is $A^{-1}=V\Sigma^{-1}U^T$
with the case where $m>n$, being referred to as the "Moore-Penrose" Inverse
& denoted as A^+.

$Ax=b$

$$\underbrace{A^+b=x}_{\text{give us the least squares solutions } m>n.}$$

$m\times n$
$m>n$.

Performed optimization for

- Single molecular { 110 eval
- multi-molecular { 310 eval.

Evaluate based on. material count.

① {
- (visualize) target design space
- trend of objective changes.
-

② - analyze the outstanding algorithms.
visualize the overall - Pareto front
- visualize the change of the design variables
shows different characteristics of diff. mes
twe the input.

③ {
- Count the material evaluated by all the algorithm.

- benchmarked by Sobol to show how different algorithms tailor properties along and/or reconstruct des. space.

mult. compare new value

Week9

* truncated vs. selected SVD

$$A^+ = \sum_i \frac{u_i^T b}{\sigma_i} v_i .$$

Selective SVD

$$x_{reg} = \sum_{i=1}^{n} \underbrace{\varphi_\alpha(\sigma_i^2)}_{\begin{cases} 1 & \sigma_i^2 > \alpha \\ 0 & \sigma_i^2 \leq \alpha \end{cases}} \frac{u^T b}{\sigma_i} v_i$$

Deterministic Error Analysis.

$$x_{reg} = \sum_{i=1}^{n} \varphi_\alpha(\sigma_i^2) \frac{u_i^T b}{\sigma_i} v_i$$

strictly positive regularization Param.

$Ax = b$ = Forward Problem.

$x_{reg} = R_\alpha b \rightarrow A^{-1}$. regularized inverse prob.

$\alpha \to 0 \Rightarrow R_\alpha = A^{-1}$.

$D\Sigma A$.

$$e_{reg} = x_{reg} - x_{exact} = e_{reg}^{trunc} + e_{reg}^{noise}$$

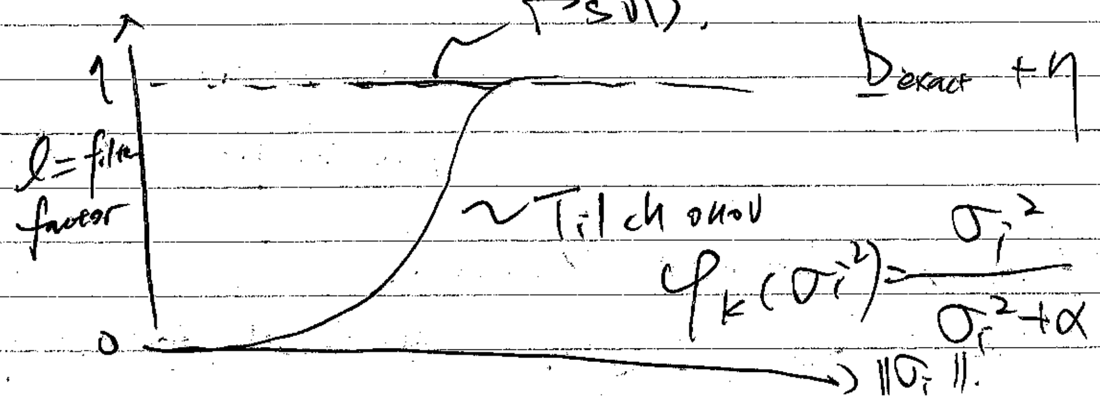
$$R_\alpha \doteq \sum_{i=1}^{n} \varphi_\alpha(\sigma_i^2) \frac{u^T b}{\sigma_i}$$

↳ "Regularization operator"

$$e_{reg}^{trunc} = \sum_{i=1}^{n} \left(\varphi_\alpha(\sigma_i^2) - 1\right) v_i^T x_{exact} v_i \quad (*)$$

$$e_{reg}^{noise} \doteq R_\alpha \eta = \sum_{i=1}^{n} \varphi_\alpha(\sigma_i^2)\, \sigma_i^{-1}(u_i^T \eta) v_i$$

$\underline{b}_{exact} + \eta = \underline{b}$



It can be shown that truncated SVD, along with Tikhonov reg. result in Inv. Sol'ns having $e_{reg} \to 0$ as $\delta = 0$

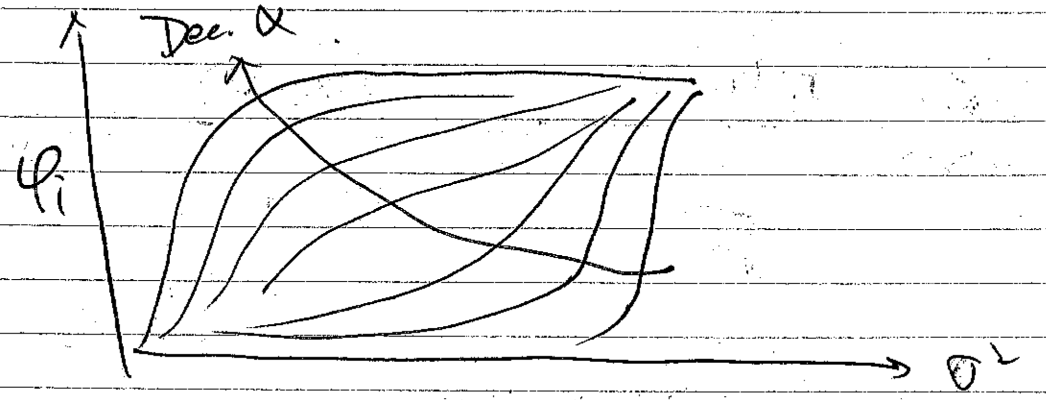
$\delta = \|\eta\|$

We now demonstrate this property for the case of Tikhonov Reg.

$$\varphi_\alpha(\sigma_i^2) = \frac{\sigma_i^2}{\sigma_i^2 + \alpha}$$

and so, for any fixed SV σ_i, we have that the filter factor

$$\varphi_\alpha(\sigma_i^2) \to 1 \quad \text{as} \quad \alpha \to 0$$



With this in mind, Eqn (*) reveals

$e_{reg}^{trunc} \to 0$ as $\alpha \to 0$.

We now turn attention to the effects of noise amplification by R_α on e_{reg}^{noise}

To begin we introduce a useful bound,

$$\varphi_\alpha(\sigma_i^2)\,\sigma_i^{-1} \underset{\Delta}{\le} \alpha^{-\frac{1}{2}}$$

In order to show the validity of this bound, we notice that $\varphi_\alpha(\sigma_i)\,\sigma_i^{+}$ is "dominated" by $\frac{1}{\sqrt{\alpha}}$

$$\lim_{\alpha \to \infty} \frac{\frac{\sigma_i}{\sigma_i + \alpha}}{\frac{1}{\sqrt{\alpha}}} = \frac{\overset{\sim \text{order } \frac{1}{2}}{\sqrt{\alpha_i}\,\sigma_i}}{\sigma_i^2 + \underset{\uparrow \text{ order } 1}{\alpha}} = 0$$

So "at infinity" this bound hold, we now show that the two functions do not cross $(0, \infty)$.

To do this, we form a function from the difference of our two terms. & then search for real roots of the equation:

$$\frac{\sigma_i}{\sigma_i^2 + \alpha} = \frac{1}{\sqrt{\alpha}}$$

$$\alpha^2 + \sigma_i^2 \alpha + \sigma_i^4 = 0$$

$$r_1, r_2 = \frac{\sigma_i^2 \pm \sqrt{-3\sigma_i^9}}{2}$$ → there are no real roots

We now employ this bound, that is related to our filter factors, to arrive at a bound for e_{reg}^{noise}. We begin by measuring the size of noise error

$$\|e_{reg}^{noise}\| = \Big\| \sum_{i=1}^{n} \underbrace{\varphi_\alpha(\sigma_i^2)\sigma_i^{-1}}_{\leq \frac{1}{\sqrt{\alpha}}} \underbrace{(u_i^T\eta)}_{\|u\|=1,\ \|\eta\|=\delta} \underbrace{v_i}_{\|v\|=1} \Big\|$$

$$\Rightarrow \underbrace{\|\bar{e}_{reg}^{noise}\|}_{\text{component-wise error}} \leq \alpha^{-\frac{1}{2}}\delta \qquad (**)$$

Using this bound, we now show that if we select $\alpha = \delta^P$, with $P < 2$, then we obtain one of our desired properties. (i.e. for one component of e_{reg}).

Let $\alpha = \delta^P$, then $\|\bar{e}_{reg}^{noise}\| = \delta^{-\frac{P}{2}}\delta^{\frac{2}{2}} = \delta^{\frac{2-P}{2}}$

To keep things from blowing up, (to not have things blow up as $\delta \to 0$.

$$\Rightarrow \frac{2-P}{2} > 0 \Rightarrow P < 2.$$

$(P<2)$

When this is true,

$\Rightarrow \|\bar{e}_{reg}^{noise}\| \to 0$ as $\delta \to 0$.

If, in addition, we restrict $P > 0$, then we preserve the property that as $\alpha = \delta^P \to 0$, $e_{reg}^{trunc.} \to 0$, $e_{reg} \to 0$ as $\delta \to 0$.

$R_\alpha \to A^{-1}$

$R_\alpha b \to x_{exact}$.

Week 9.

Deterministic Error Analysis.

$b_{exact} + \eta$

$Ax = b$ — measure

system — inv soln.

$$e_{reg} := x_{reg} - x_{exact}.$$

$$= e_{reg}^{trunc.} + e_{reg}^{noise}. \quad R_\alpha \approx A^{-1}.$$

(Regularization operator.

in the case of Tikhnov $\left\{ \begin{array}{l} e_{reg}^{trunc} \to 0 \quad \text{as } \delta \to 0 \\ e_{reg}^{noise} \to 0 \quad \text{as } \delta \to 0. \quad \|\eta\| = \delta \end{array} \right.$

$\alpha = \delta^p,$

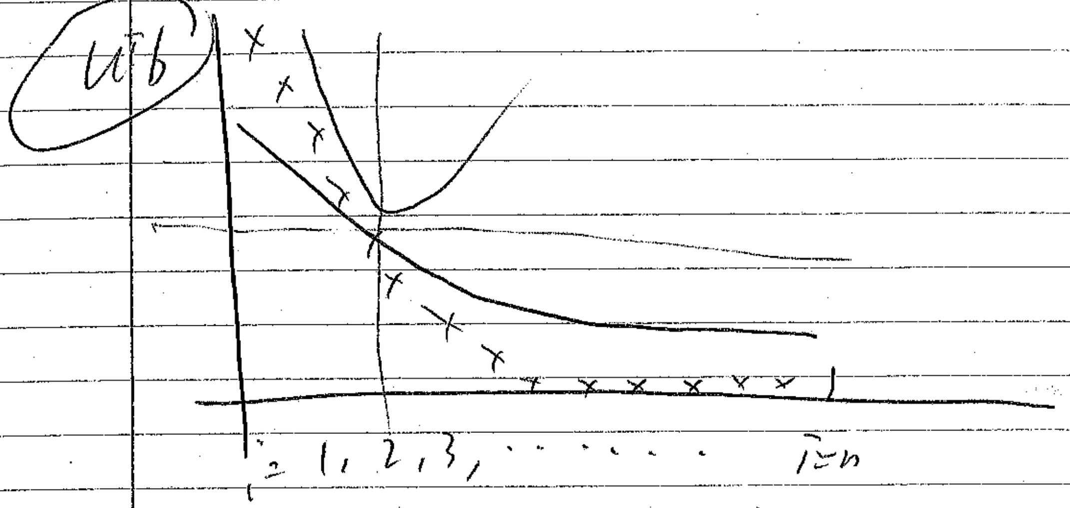
$p \in (0, 2)$

- Rates of Convergence

Consider truncated SVD with

$\delta \geq \sigma_n^2$ (otherwise why bother with regularization

RHS coeffs.



and assume the "Range Condition".

that $x_{exact} = A^T z, \quad z \in \mathbb{R}^n$

i.e. $x_{exact} \in \mathcal{R}_{A^T}$.

(related to the sum cond. by SVD

Since $$\left|(A^T z)^T v_i\right| = \left|z^T A v_i\right| \overset{\text{by SVD}}{=} \left|z^T u_i \sigma_i v_i^T v_i\right|$$

$$= \underbrace{\sigma_i \left|z^T u_i\right|}_{x_{exact} v_i}$$

then, using $\|v_i^T\| = 1$

Recall :

$$\|e_{reg}^{trunc}\| = \sum_{i=1}^{n} (\varphi_\alpha(\sigma_i^2) - 1) u_i^T x_{exact} v_i$$

$$\|e_{reg}^{trunc}\|^2 = \sum_{i=1}^{n} (\varphi_\alpha(\sigma_i^2) - 1)^2 \sigma_i^2 |z^T u_i|^2$$

$$\leq \max_{1 \leq i \leq n} (\varphi_\alpha(\sigma_i^2) - 1)^2 \sigma_i^2 \|z\|^2$$

"upper bound"

We now let $\varphi_\alpha(\sigma_i^2))$ be equal to its bound: $\sigma_i \alpha^{-\frac{1}{2}}$, and so

$$(\sigma_i \alpha^{-\frac{1}{2}} - 1)^2 \sigma_i^2 \|z\|^2$$

$$\underbrace{\sigma_i \alpha^{-1} = 2\sigma_i \alpha^{-\frac{1}{2}} + 1) \sigma_i^2}\ \|z\|^2$$

$$\lim_{\alpha \to \infty} \frac{\text{▨}}{\alpha} = 0 \Rightarrow \alpha$$

thus, bound:

$$\|e_{reg}^{trunc}\|^2 \leq \alpha \|z\|^2, \quad z \in \mathbb{R}^n$$

$$\|e_{reg}^{noise}\| \leq \alpha^{-\frac{1}{2}} \delta \quad (**)$$

Combining this with (**), our earlier bound on the influence of noise, we get

$$\|e_{reg}\| \leq \underbrace{\alpha^{+\frac{1}{2}} \|z\|}_{\text{①}} + \underbrace{\alpha^{-\frac{1}{2}} \delta}_{\text{②}}$$

This bound on regularization error can be minimized w.r.t. α.

$$\frac{\partial}{\partial \alpha} (\alpha^{-\frac{1}{2}} \|z\| + \alpha^{\frac{1}{2}} \delta) = 0$$

$$\frac{1}{2}\alpha^{-\frac{1}{2}}\|z\| - \frac{1}{2}\alpha^{-\frac{3}{2}}\delta = 0.$$

and so,

$$\frac{1}{2}\alpha^{-\frac{1}{2}}\|z\| = \frac{1}{2}\alpha^{-3/2}\delta$$

$$\alpha^{-\frac{1}{2}}\alpha^{\frac{3}{2}} = \alpha = \frac{\delta}{\|z\|} \leftarrow \text{subs. ①\&②}$$

yields:

$$①: \sqrt{\frac{\delta}{\|z\|}}\,\|z\| = \sqrt{\delta}\,\sqrt{\|z\|}.$$

$$②: \frac{\delta}{\sqrt{\frac{\delta}{\|z\|}}} = \sqrt{\delta}\,\sqrt{\|z\|}$$

$\oplus \leftrightarrow 2\|z\|^{1/2}\delta^{1/2}$

and so $\|e_{reg}\| \le 2\|z\|^{1/2}\delta^{1/2}$; thus

we see that $\|e_{reg}\| = \mathcal{O}(\sqrt{\delta})$ as $\delta \to 0$

we conclude the truncated SVD is "order optimal", when $x_{exact} \in R_{A^T}$

bounded by a const, times least error, i.e., 0

This also holds for "Tikhonov regularization".

A little Regularization theory

$\forall g \in R_A$ ← range $\exists!\ R_*(g) \in \mathcal{H}_1$.

g.

$$\int k(x,y)\, f(y)\, dy = g(x)$$

for which $A(R_*(g)) = g$, i.e. $R_* = A^+$.

the Moore-Penrose Inverse

$$A^+ = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i$$

We now consider a family of regularization operators, $R_\alpha : \mathcal{H}_2 \to \mathcal{H}_1$

where α is a regularization parameter (e.g. the α's in our filter-functions) which lies in some index set, I..

Definition: $\{R_\alpha\}_{\alpha \in I}$ is a regularization scheme that converges to R^* if:

1) for all $\forall \alpha \in I$, the resulting R_α is a continuous operator,

2) given any $g \in R_A$ for any sequence $\{g_n\} \in \mathcal{H}_2$ that converges to g. one can pick a sequence, $\{\alpha_n\} \subset I$, s.t. $R_\alpha(g_n) \longrightarrow R_*(g)$ as $n \to \infty$.

The regularization scheme is called "linear" if each of the R_α are (bounded) linear operator. Our filter factor regularization schemes. one convergence by this definition since

$$(**) \quad R_\alpha(g) = \sum_j \frac{\varphi_\alpha(\sigma_n^2)}{\sigma_j} \langle g, u_j \rangle_{\mathcal{H}_2} v_j$$

$\alpha \in I = (0, \infty)$

converges to $R_* = A^+$

We can see that (**)

1. $\|R_\alpha\| = \sup_j \frac{\varphi(\sigma_i^2)}{\sigma_j}$

Suppose that $g \in R_A$., and that $g_n \in \mathcal{H}_2$, $\delta_n > 0$, satisfy the

2. relation $\|g_n - g\| \le \delta_n$

Using these two results, along with the

triangle inequality, we obtain

$$\|R_{\alpha_n} g_n - R_* g\| \leq \|R_{\alpha_n} g - R_* g\| + \|R_{\alpha_n}\| \quad (\#)$$

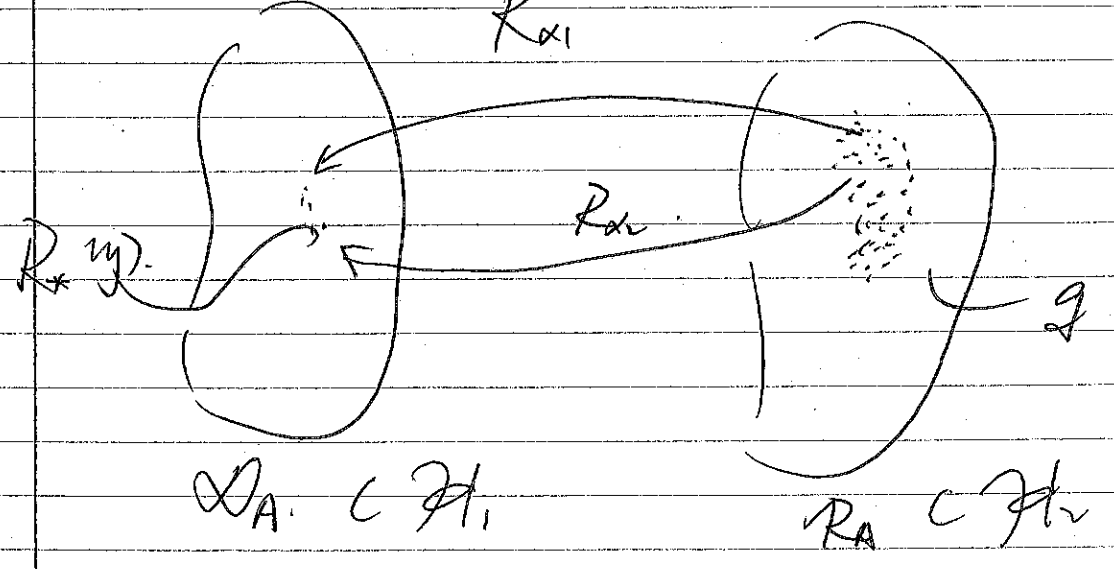
The following theorem establishes conditions that guarantee that we can select $\alpha = \alpha(\delta)$ so that both terms on the RHS ~~(**)~~ (#) converge to zero $\delta_n \to 0$ we let $\alpha_* = 0$ denote the filter functions Parameter value yielding R_*.

Week 9/10

Definition: $\{R_\alpha\}_{\alpha \in I}$ is a regularization scheme that converges R_*. if

1) $\forall\ \alpha \in I$, the resulting R_α is a continuous operator, and

2). given any $g \in R_A$ for any sequence $\{g_n\} \subset \mathcal{H}_2$, that converges to g, one can pick a sequence, $\{\alpha_n\} \in I$, s.t. $R_{\alpha_n} \to R_*(g)$ as $n \to \infty$



From Boundedness & application of triangle inequality.

$$\|\underbrace{R_{\alpha_n} g_n}_{\text{approx}} - \underbrace{R_* g}_{\text{best possible}}\| \le \|R_{\alpha_n} g - R_* g\| + \|R_{\alpha_n}\| \delta_n \qquad (\ddagger)$$

The following theorem establishes conditions that guarantee that we can select an α as a function $\|g_n - g\| \le \delta_n$.

$$\alpha = \alpha(\delta)$$

so that both terms of $(\ddagger)$ converge to zero as $\delta_n \to 0$. We let $\alpha_* = 0$ denote the filter function parameter value yielding the desired R_*.

Theorem

Assume that for each $\alpha \in I$,

$$\sup_{\sigma > 0} \left| \frac{\varphi^2(\sigma^2)}{\sigma^2} \right| < 0$$

And that for each $\sigma > 0$, $\lim_{\alpha \to \alpha_*} \varphi_\alpha(\sigma^2) = 0$

Also, assume $\exists$ a function, $\alpha = \alpha(\delta)$, mapping R^+ into the index set, I, s.t.

$\lim_{\delta \to 0} \alpha(\delta) = \alpha_*$, and

$$\lim_{\delta \to 0} \|R_{\alpha(\delta)}\| \delta = 0, \quad \text{then}$$

$$R_\alpha(g) = \sum_j \frac{\varphi_\alpha(\sigma_j^2)}{\sigma_j} \langle g_j, u_j \rangle_{\mathcal{H}_2} v_j$$

(filter factor regularization)

(We have conditions for regularization schemes that converges to A^+)

Selecting Regularization Parameters

The Discrepancy Principle

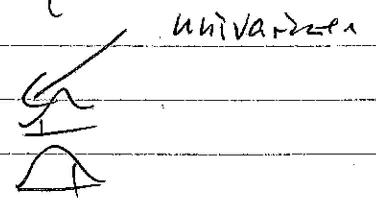
It is common that electronic sensor noise exhibit randomness that is consistent w/ Gaussian white noise. i.e. distributed normally, with all frequencies equally powerful):

observable $b = b_{exact} + \eta$

where η is a vector realization of i.i.d. Gaussian white noise.

$$b \in \mathbb{R}^n, \quad \eta \in \mathbb{R}^n, \quad \eta \sim N(0, S)$$

$$\begin{Bmatrix} (b_{exact})_1 \\ (b_{exact})_2 \\ \vdots \\ (b_{exact})_n \end{Bmatrix} + \begin{Bmatrix} \eta_1 \sim N(0, S^2) \\ \eta_2 \sim N(0, S^2) \\ \vdots \\ \eta_n \sim N(0, S^2) \end{Bmatrix} = b.$$



With this in mind, and assuming that $x_{reg} \approx x_{exact}$, then our expected residual, is dominated by the noise contribution:

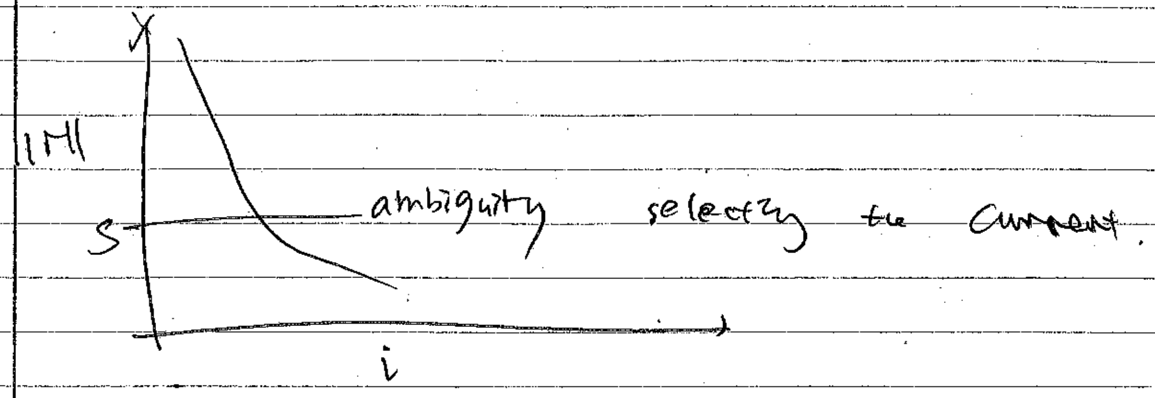
$$\mathbb{E}\left[\frac{1}{n}\|Ax_{reg} - b\|^2\right] \approx \mathbb{E}\left[\frac{1}{n}\|\eta\|^2\right] = \underbrace{S^2}_{\text{Variance}}$$

of ~~realization~~ repeated measurements

Implies repeating measurement process is repeated multiple times.

As a result, it seems useful to select a regularization parameter α, for which we have:

$$\frac{1}{n}\|\underbrace{Ax_{reg} - b}_{r \,\leftarrow\, \text{residual}}\|^2 = S^2$$



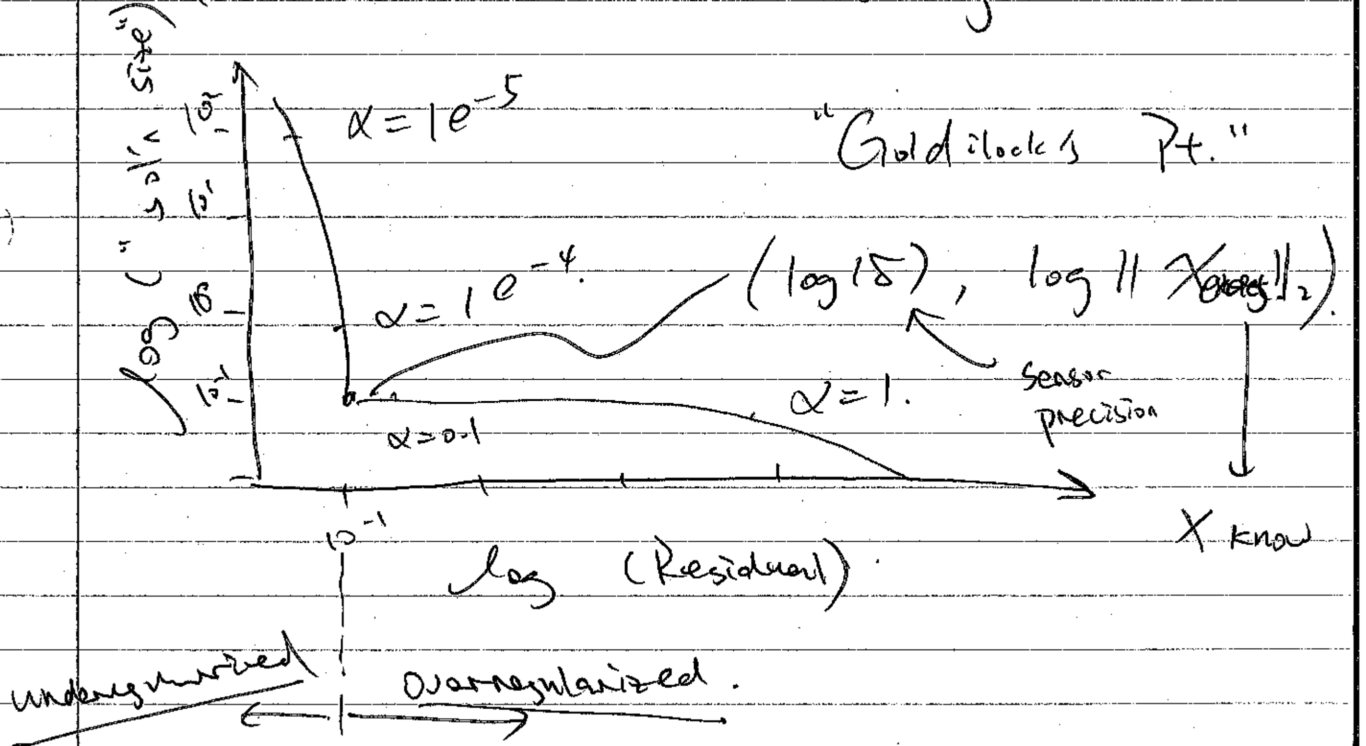
However, experience shows that the resulting inverse sol'n is quite sensitive to the parameter selection. & so in practice, ppl use this. →

$$\frac{1}{n}\|Ax_{reg} - b\| = 2\sqrt{n}\, S$$

note: This method is agnostic to the filter factor formula used, & only requires a refining algorithm for practical implementation, but does require many solve of the ~~inver~~ ~~forward~~ inverse problem.

The L-curve.

If we plot on a Log-Log axes, the sol'n norm, $\|X_{reg}\|_2$, versus the residual norm, $\|AX_{reg} - b\|_2$, then we see sth interesting:



In practice, we compete ~~the~~ curvature function of the L-curve & then compute the α maximizing the curvature.

This requires re-solving the inverse problems many times.

Real world Problems

Our discussion of Class 1 inverse problems has hinged on calculation of the SVD, which is infeasible in most practice settings because the discrete problem results in linear systems that are too large to fit into the RAM of most computers.

Additionally, the previous regularization parameter selection methods require complete resolves of the inverse prob., many times.

With all this in mind, we would like a more practical means for effecting our inverse solution, such that the new approach.

1) Avoids any matrix factorizations.

2). Exploits structured/unstructured sparsity within the discrete matrix A.

3) Involves only matrix-vector & vector-vector multiplications

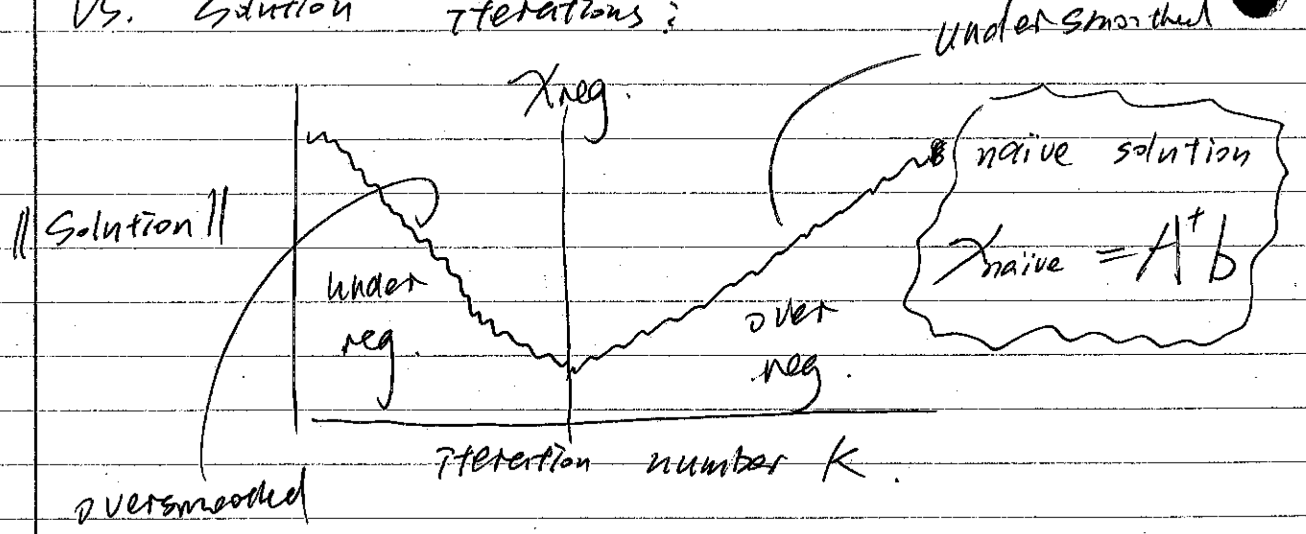
4) Allow for adjustment in our regularization parameters in a way the precludes having to start from scratch for solving our inverse problem. (helpful when problem has long run time)

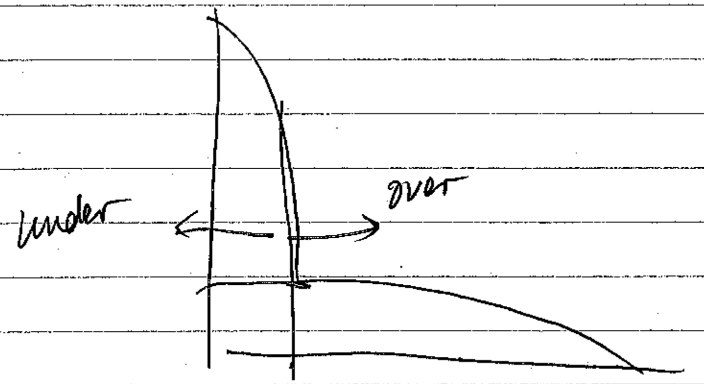
An elegant solution for this need for efficiency comes from the form of

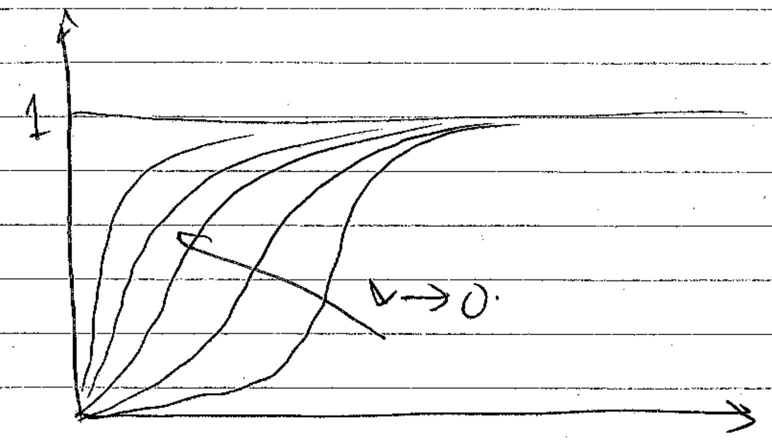
Semi-convergence iterative solution methods for linear, Algebraic systems. $Ax=b$.

(in contrast to " direct solution methods, e.g., Gauss-Jordan, Cholesky, LU, etc.)

Semiconvergent solution methods exhibit interesting behavior, in terms of solution error vs. solution iterations:







While there are many flavors of semi-convergent solvers that are useful in solving practical inverse problems we consider two particularly important examples that offer insight into (classes) two main cases of semi-convergent useful solvers.

1) Stationary methods

2). projection methods. (krylov basis)

*** "Multigrid Solvers"

Stationary ~~It~~ Method:

Landweber iteration

Basic form:

$$x^{[k+1]} = x^{[k]} + \omega A^T \overbrace{(b - Ax^{[k]})}^{\text{residual}}$$

$k = 1, 2, \dots$

and $\omega \in \mathbb{R}\left(0, \underbrace{2\|A^TA\|_2^{-1} = \frac{2}{\sigma_1^2}}_{\text{stability Limit.}}\right)$

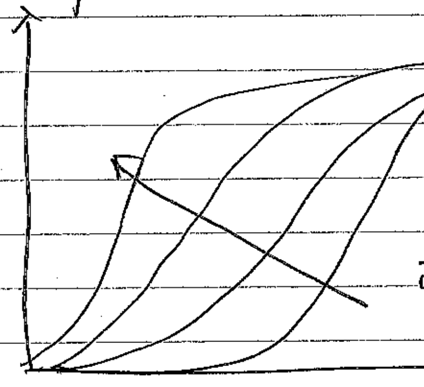
The iterate, $x^{[k]}$, can be viewed as a being a filtered SVD solution (we do this to get insight: No SVD is required here!).

$$x^{[k]} = \underbrace{V\phi^{[k]}\Sigma^{-1}U^T}_{R_{\alpha(k)}} b, \quad \phi^{[k]} = \text{diag}[\phi_1^{[k]}, \phi_2^{[k]}, \dots, \phi_n^{[k]}]$$

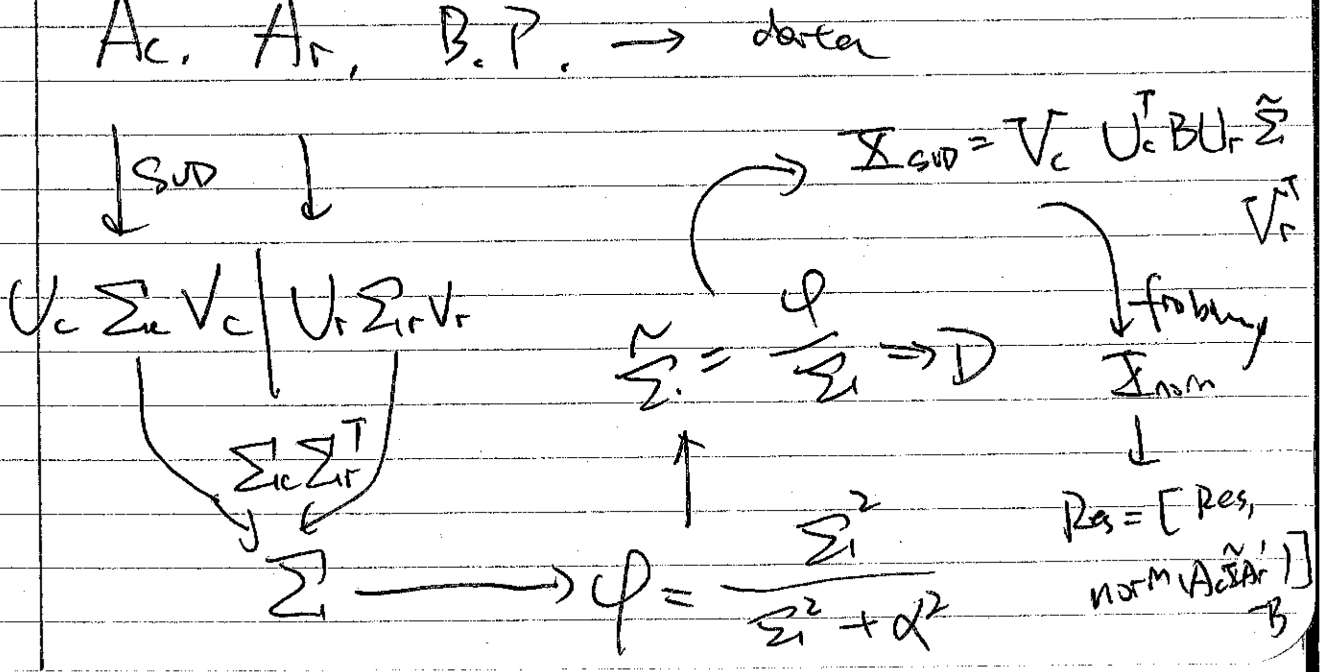
where

$$\varphi_i^{[k]} = 1 - (1 - \omega\sigma_i^2)^k, \quad i = 1, 2, \dots, n.$$

and it can be shown that for small σ_is, we have $\varphi_i^{[k]} \approx k\omega\sigma_i^2$; thus "Landweber filter factors" decay at the same rate as Tikhonov counterparts.



increasing [k] => ultimately ending @ A^+b.



Bayes Thm

$$P_{\vec{\Theta}|\vec{Y}}(\vec{\theta}|\vec{y}) = \frac{P_{\vec{Y}|\vec{\Theta}}(\vec{y}|\vec{\theta})\,P_{\vec{\Theta}}(\vec{\theta})}{P_{\vec{Y}}(\vec{y})}$$

$$\int_{\vec{\theta}\in\mathbb{R}^n} P_{\vec{Y}|\vec{\Theta}}(\vec{y}|\vec{\theta})\,P_{\vec{\Theta}}(\vec{\theta})\,d\theta$$

hard to evaluate, high dimensional integral.

The issue with the high dim. Int. Bayes theorem motivated the Landmark work of Hastings (1972) when he built from earlier ideas of Metropolis, work at LANL in 1940s.

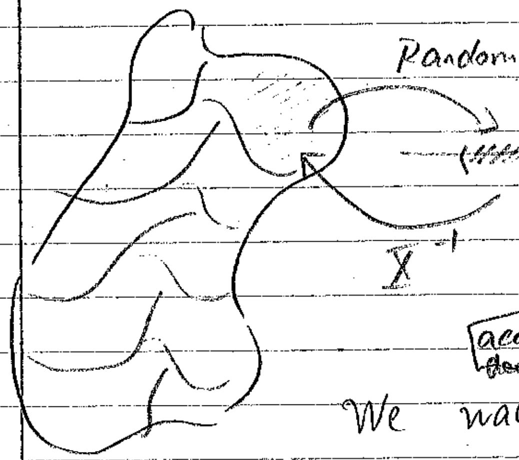
In our class-2 inverse problems, the integral is taken over the parameter space in stimulating our model $\mathcal{M}(\vec{x};\vec{\theta})$, $\vec{\theta}\in\mathbb{R}^n$

If "n" is large then m-point Quadrature rule becomes unwieldy; requiring m^n quadrature points!! Typically, also, a quadrature rule requires some prior knowledge of the support of the function being integrated unknown in the case of our posterior distri.

In response to these difficulties, Building on the vital results of the Metropolis Hastings; we take an alternative approach Instead of evaluating probability density of a given point, we let the density function itself determine a set of points. (call these "samples") that will support the posterior distribution. these pts are employed in approximating our integral. leading to "Markov Chain Monte Carlo" (MCMC)

MCMC Methods

Let μ denote a probability measure over $\mathbb{R}^n$. & Let f be a scalar or vector valued function that is integral Random variable over $\mathbb{R}^n$ w.r.t. the ~~([illegible])~~ measure, μ, that is



$$\overset{\Downarrow}{\text{CDF}} \quad f \in L^1(\mu(dx))$$

accumulated density function

We want to estimate the integral of "f" w.r.t. the measure μ.

We mention before that in numerical quadrature one defines a set of support pts. $x_j \in \mathbb{R}^N$, $i \le j \le N$, along with corresponding weights, w_j, in order to obtain

$$\int_{\mathbb{R}^N} f(x)\,\mu(dx) \approx \sum_{j=1}^{n} w_j f(x_j)$$

In contrast, MC method randomly generate the x_j using some probability density.

And the weights are then determined using our measure, $\mu \curvearrowright \text{CDF}, F_X$.

In the ideal case, $X \sim \mu$, and then we obtain the "ergodic average" approximation,

$$(*) \quad \int_{\mathbb{R}^N} f(x)\,\mu(dx) = \mathbb{E}(f(x)) \approx \frac{1}{n}\sum_{j=1}^{n} f(x_i)$$

The MCMC method offers a systematic means for generating samples that build up a useful ergodic average – the probability density determine the frequency of samples.

We will devise a scheme such that we generate a sample ensemble s.t. (*) holds.

(we don't know the CDF)

Let $\mathcal{B} = \mathcal{B}(\mathbb{R}^N)$ denote the Borel set over $\mathbb{R}^N$, A mapping $P : \mathbb{R}^N \times \mathcal{B} \to [0,1]$. is called a "probability transition kernel", if

1) for each $B \in \mathcal{B}$, the mapping from $\mathbb{R}^N$ into $[0,1]$, $x \mapsto P(x, B)$, is a measurable function

2). for each $x \in \mathbb{R}^N$, the mapping from $\mathcal{B}$ into $[0,1]$, $B \mapsto P(x, B)$ is a probability distribution.

A In "discrete-time stochastic process" is an ordered set, $\{x_j\}_{j=1}^{\infty}$, of random variable $X_j \in \mathbb{R}^N$.

A "Time-homogeneous Markov chain" with "transition kernel", P, is a discrete time stochastic process, $\{x_j\}_{j=1}^{\infty}$, with properties,

$$\mu_{X_{j+1}}(B_{j+1} | x_1, x_2, \dots, x_j) =$$

$$\mu_{X_{j+1}}(B_{j+1} | x_j),$$

$$\Downarrow$$

time homogeneous

$$= P(x_j, B_{j+1})$$

①, the probability them. $X_{j+1} \in B_{j+1}$, Conditioned on obs. $X_1 = x_1$, $X_2 = x_2$, ... $X_j = x_j$, equals the prob. conditioned on $X_j = x_j$, alone.

② "time is homogeneous.

in the sense the dependence of adjacent moments in time does not evolve. — it is stationary. i.e. prob. transition kernel, P, does not depend on time j.

② is also indicating the relationship between our transition probs & the file [illegible]

Cof μ, we build up knowledge on μ,

we want all these! How?

We know generate transition and that propagates k steps forward in finite times

$$P^{(k)}(x_j, B_{j+k}) = \underbrace{\mu_k(B_{j+k} | X_j)}$$

prob. prob. meaning.

Uts – myc ceo

$$= \int_{\mathbb{R}^n}^{2011} (X + B_{j+k}) \underbrace{P^k(x_j, dx_{j+1})}_{b\,x_2}$$

Where it is understood that "p"(x_j, B_{j+1}) $P(x_j, Y_j)$. In particular if μ_x denotes the [illegible] [illegible], then the distribution.

$$\mu_{x_{j+1}}(B_{j+1}) = \underbrace{\mu_{x_j}}_{\text{start here}} \underbrace{\overset{x_j \text{ is simplified}}{P(B_{j+1})}}_{\text{we build up knowledge of } X_{j+1} \text{ by repeatedly applying trans. kernel}} = \int_{\mathbb{R}^n} P(x_j, B_{j+1}) \mu_{x_j}(dx_j)$$

(B_{j+1})

$\hookrightarrow$

Supporting concepts

"Probability transition kernel" → if I'm at some state x_j, whats the prob. of moving → $B_{j+1} \in \mathcal{B}$

"discrete time stochastic process", … $\{X_j\}$

"Time homogeneous Markov chain" with transition kernel "p".

$$\mu_{X_{j+1}}(B_{j+1} | x_1, x_2, \dots, x_j) = \mu_{X_{j+1}}(B_{j+1} | x_j)$$

$$= P(X_j, B_{j+1})$$

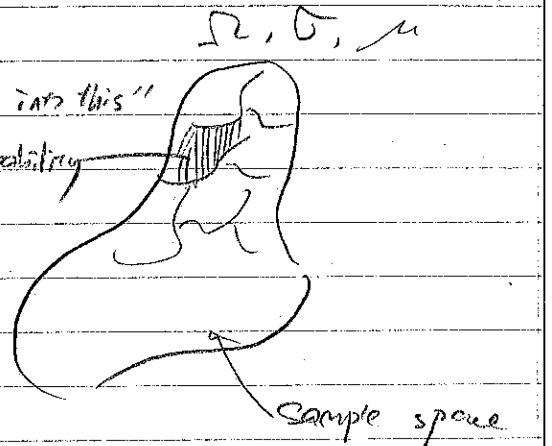
$$\mu_{X_{j+1}}(B_{j+1}) = \underbrace{\mu_{X_j}}_{\text{Start here}} \overset{X_j \text{ implied.}}{P(B_{j+1})} = \int_{R^N} P(x_j, B_{j+1}) \mu_{x_j}(dx)$$

we build up our knowledge of X_{j+1} by repeated repeatly applying our trans kernel

μ is an "invariant measure" of $P(x_j, B_{j+1})$ if $\mu P = \mu$.

Definition → irredeccaisility.

Given prob. measure μ, the probability transition kernel, P, is irreducible (w.r.t. μ), if for each $x \in \mathbb{R}^N$, & $B \in \mathcal{B}$, with probability greater than 0: $\mu(B) > 0$, then there exists an integer, k, such that $P^{(k)}(x, B) > 0$, "fill into this"



i.e. regardless of the starting point, the Markov chain are generated by the transition kernel, P, visits with positive probability any set of positive measure.

Definition Let P be an irreducible prob. trans. kernel. we say that P is "periodic", if for some integer, $m \geq 2$, there is a set of disjoint, no empty, opensets. $\{E_1, E_2, \dots, E_m\} \in \mathbb{R}^N$ s.t. $\forall_j = 1, 2, \dots, m$, & $\forall x \in E_j$. $P(x, E_{j+1 (\text{mod } m)}) = 1$

that is a periodic prob. trans. kernel, generates a Markov chain that includes a periodically loop forever. a non-periodic

Theorem Let μ be prob. measure in $\mathbb{R}^N$, & $\{X_j\}$ the time homogeneous Markov chain with probability transition kernel, P. Assume μ is an invariant measure of the probability transition kernel, P, $\overset{\&}{\rightarrow}$ that P is irreducible and aperiodic. Then for $\forall x \in \mathbb{R}^N$, we have:

$$\lim_{n\to\infty} P^{(*)}(x,B) = \mu(B), \quad \forall B \in \mathcal{B}$$

and for $f \in L^1(\mu(dx))$

$$\underbrace{\lim_{n\to\infty} \frac{1}{n}\sum_{j=1}^{n} f(X_j) = \int_{\mathbb{R}^N} f(x)\,\mu(dx) \quad (a.s.)}_{\text{"Erogdicity property of Monte Carlo integration"}}$$

The foregoing thm. explains how to properly explore a given prob. density func.: construct an invariant, aperiodic, irreducible, prob. trans. kernel, P, & draw a sequence of samples $(x_1, x_2, \ldots)$ using P to form a realization of a Markov chain

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We now pursue a suitable MCMC prob. trans. kernel. We begin by letting μ denote the "target prob. distrib." (i.e., the one we want to sufficiently approximate) in $\mathbb{R}^N$ that we want to explore with a suitable sampling algorithm. In support of this, we require $P(x,B)$ s.t. μ is its invariant measure. Let P denote any prob. trans. kernel. When $x \in \mathbb{R}^N$ is given, we can have that the kernel proposes a move to $y \in \mathbb{R}^N$, or it purposes no such move. thus we split the kernel into two parts:

$$P(x,B) = \int_B K(x,y)\,dy + r(x)\chi_B(x)$$

"characteristic function" of set $B \in \mathcal{B}$

$K(x,y) \geq 0$ is a density function & we can think of $K(x,y)\,dy$ as being the prob. of a move from x to the infinitesimal set, dy, @ y, while $r(x) \geq 0$ is the probability that we stay @ x.

The characteristic function χ_B, of B appears since if $x \in B$, then the only way for x to "reach" B, is through a move.

The condition $P(x, \mathbb{R}^n) = 1$ implies.

$$r(x) = 1 - \int_B K(x,y)\,dy.$$

So we can get PDF from our CDF

we assume μ is absolutely continuous, w.r.t. the Lebesgue measure, $\mu(dx) = \underbrace{\pi(x)\,dx}$

Lebesgue measure on the $\mathcal{B}_n$ algebra where the random vars x.

and in order for $\pi(x)\,dx$ to be a measure of P, we have to satisfy the identity.

$$\mu P(B) = \int_{\mathbb{R}^n} \underbrace{\left(\int_B K(x,y)\,dy + r(x)\chi_B(x)\right)}_{P(x,B)} \pi(x)\,dx$$

$$= \int_B \left(\int_{\mathbb{R}^n} \pi(x)\,K(x,y)\,dx + r(y)\,\pi(y)\right) dy$$

$$= \int_B \pi(y)\,dy$$ implying that

$\forall B$ $$\pi(y)\,(1 - r(y)) = \int_{\mathbb{R}^n} \pi(x)\,K(x,y)\,dx$$

this leads to "detailed Balance"

$$\int_{\mathbb{R}^N} \pi(y)\, k(y,x)\, dy = \int_{\mathbb{R}^N} \pi(x)\, k(x,y)\, dx \quad (*)$$

& so if k satisfies detailed balance, then we have the

$$\pi(y)\, k(y,x) = \pi(x)\, k(x,y) \quad (**)$$

Conditions $(*)$ & $(**)$ are our starting pt. for constructing the Markov chain trans. kernel req'd for MCMC sampling

Detailed Balance.

$$\pi(y)\, k(y,x) = \pi(x)\, k(x,y)$$
$$\Downarrow$$

stationary point → constructing MC transitioning kernel for MCMC sampling

In pursuit of this transition kernel that satisfies detailed Balance let $q : \mathbb{R}^n, \mathbb{R}^n \to \mathbb{R}_+$ be given s.t. $\int q(x,y)\,dy = 1$. This kernel is called the "proposal distri." ("Candidate generating kernel").

& it can be used to generate a prob. trans. kernel: $Q(x,A) = \int_A q(x,y)\,dy$

If q satisfies detailed then we set $K(x,y) = q(x,y)$, & $r(x) = 0$; otherwise we correct the kernel using multip. factor

$$k(x,y) = \underbrace{\alpha(x,y)}_{\text{Correction}} \; q(x,y) \qquad (\#)$$

Assume that, for some $x, y \in \mathbb{R}^n$, instead of detailed balance, we have

$$\pi(y)\, q(y,x) < \pi(x)\, q(x,y)$$

In such a case, we can choose direction $\alpha(x,y)$, s.t.

$$\pi(y)\,\alpha(y,x)\, q(y,x) = \pi(x)\,\alpha(x,y)\, q(x,y)$$

which is achieved if we set

$$\alpha(y,x) = 1 \quad \text{and} \quad \alpha(x,y) = \frac{\pi(y)\, q(y,x)}{\pi(x)\, q(x,y)} < 1.$$

(#) satisfies detailed balance

We can write down our metropolis Hastings Transition Kernel

$$\alpha(x,y) = \min\left[1, \frac{\pi(y)\, q(y,x)}{\pi(x)\, q(x,y)}\right],$$

1. Select an initial $x \in \mathbb{R}^n$ & set $k=1$.
2. Draw $y \in \mathbb{R}^n$ from proposed distribution $q(x_k, y)$ & compute "acceptance ratio",

$$\alpha(x_k, y) = \min\left[1, \frac{\pi(y)\, q(y, x_k)}{\pi(x_k)\, q(x_k, y)}\right]$$

3. Draw $t \sim U[0,1]$.
4. If $\alpha(x_k, y) \geq t$, then set $x_{k+1} = y$.
   Else set $x_{k+1} = x_k$.
5. If $k =$ the desired sample size, then stop.
   Else increase $k \to k+1$ & go to 2.

$\boxed{\text{4-3\%}\quad \text{rejection model}}$

Additional Course Notes : Inverse Modeling

Math Inverse Modeling

Stochastic Inversion.

- Encode uncertainty.

apply to class 2 inverse problems. applies statistical methods, in a quest for information concerning some "quantity of interest". - QOI. Said another way, the aim of stochastic inversion is to extract information and quantify its uncertainty using methods that leverange available knowledge about the measurement process, as well as information models for the QOI's, that are available prior to measurement.

Our program for statistical inversion is found on three principles.

1). All variables within our model $\mathcal{M}[(\vec{x},t);\theta]$ are treated as "Random Variables".

2). The associated randomness may be quantified & used to gauge information contained, therein using probability (function) measures,

3). The solution of the inverse problem is the "posterior probability Distribution".

Item 3) represents a stark contrast to the traditional regularization methods, previously discussed;

Regularization methods produce a single estimate of the Quantity OI, while our Stochastic methods will furnish distributions of the QOIs ... each with the own probability" (so the speak).

Statistical estimation theory.

$\prod_{i=1}^{n} i = 1\times2\times\dots\times n = n!$

In statistical modeling & some system response. We conceive of some space that contains all the possible system responses - the "Sample space". This sample space is then covered with an "event space" (σ- algebra). comprising all measurable outcomes of interest that can occur on our sample space; each with its own probability occurrence that is furnished with some probability measure.

Math statistics, it is common to denote

a "Random Variable" (i.e., a map from the physical sample space to the space of the reals) with a Capital letter, & use a lower case letter to denote realization (sample) of the random variable; If $X: S \to \mathbb{R}$ is a random variable, then $x \in \mathbb{R}$ (meaning the realization sample is taken from the range of X)

By $\{X \le x\}$ we $\overset{\text{mean}}{\text{have}}$:

$$\{s \in S \mid X(s) \le x\}$$

Definition A "probability space" is the triple

$$(\underset{\substack{\text{Sample} \\ \text{space}}}{S}, \underset{\substack{\text{event} \\ \text{space}}}{\beta}, \underset{\text{probability measure}}{P})$$

Probability measure: $P: \beta \to \mathbb{R}_+$

with $P(\phi)=0$ & $P(S)=1$.

$$P(\cup_i b_i) = \sum_i P(b_i)$$

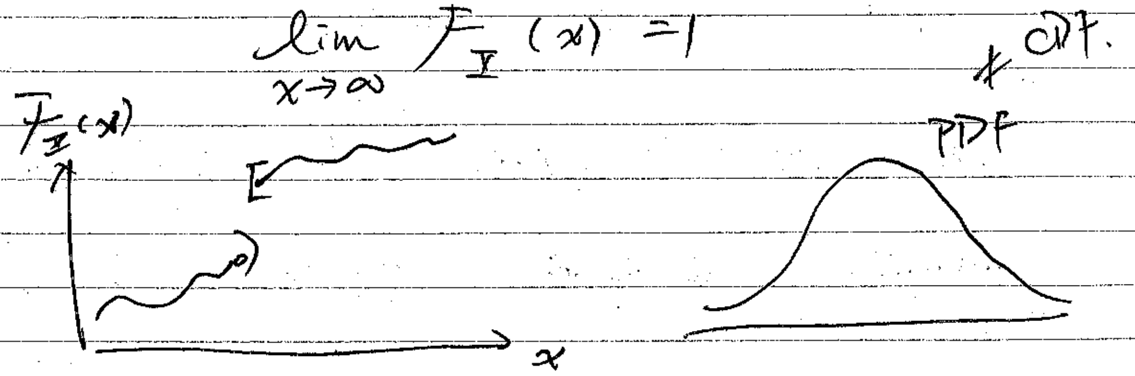
for any dis. colle. of $b_i \in \beta$.

A random variable is a "measurable function", $X: S \to \mathbb{R}$, having a "cumulative distribution function". $F_X(x) = P(X \le x)$, $x \in \mathbb{R}$.

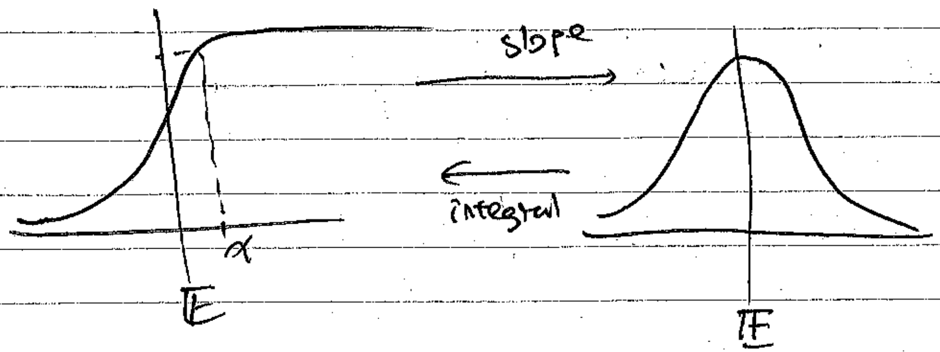
non-decreasing & ~~accumulative~~ right continuous function. &

Satisfies $\lim\limits_{x \to \infty} F_X(x) = 0$.

$$\lim_{x \to \infty} F_X(x) = 1$$



CDF



Definition. Random variable, X, is called "discrete" if there exist ~~a~~ countable sets $\{x_i\} \subset \mathbb{R}$ and $\{P_i\} \subset \mathbb{R}_+$, s.t. $P_i = \mathbb{P}\{X = x_i\} > 0$, for each i, & $\sum_i P_i = 1$. Our probability function, in this case is called the "probability mass" function, that is a real-valued, discretely supported function, s.t.

$$P_X(x) = \begin{cases} P_i, & \text{if } x = x_i,\ i = 1, 2, \dots, \\ 0, & \text{otherwise} \end{cases}$$

The x_i are points of discontinuity in Cumulative distripution function (CDF), F_X:

$$F_X(x) = \sum_{\{i \mid x_i \le x\}} P_X(x_i) = \int_{-\infty}^{x} \left(\sum_i P_X(x_i)\,\delta(u - x_i)\, du\right)$$

where $\delta(\cdot)$ is now the Dirac delta distribution

– Discussion on continuous Random Variables.

Definition Random Variables.

→ X is called continuous if its cumulative distribution function F_X is absolutely continuous.

In this case,

$$F_X(x) = \int_{-\infty}^{\infty} P_X(u)\, du$$

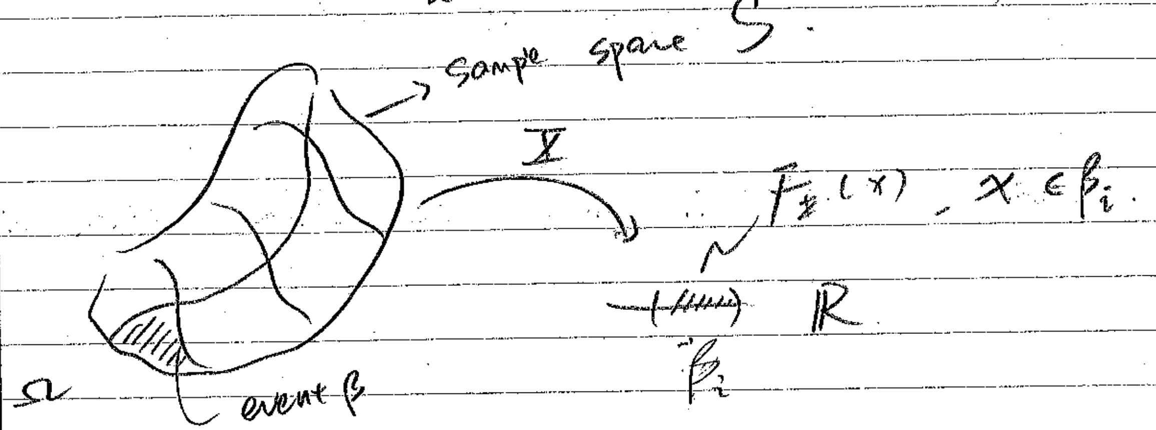
and the derivation

"Probability Density function for X"

$$\rightarrow P_X(x) = \frac{d F_X}{d x}$$

Definition. The "mean" or "Expected Value" of a random variable, X, is given by the linear operator

$$\mathbb{E}(X) = \int_{-\infty}^{\infty} x \, dF_X(x).$$



while is the discrete case

$$dF_X(x) = P_X(x_i)\,\delta(x - x_i)$$

$$\Rightarrow \mathbb{E}(x) = \sum_i x_i P_X(x_i).$$

Example : coin toss

Sample space, for a fair coin is

with $P(\Phi) = 0$, $P(S) = 1$, $S = \{\underset{\text{tails}}{T}, \underset{\text{heads}}{H}\}$

$P(\{H\}) = \frac{1}{2}$, $P(\{T\}) = \frac{1}{2}$

We define a random variable, $X : S \to \mathbb{R}$

s.t. $X(T) = 0$ and $X(H) = 1$, that is

discrete with probability mass function:

$$P_X(x) = \begin{cases} \frac{1}{2}, & \text{if } x = 0, 1. \\ 0, & \text{otherwise} \end{cases}$$

$\mathbb{E}(X) = \frac{1}{2}$.

Definition Two random variables, X & Y, are "jointly distributed" if they are both defined on the same probability space (S, β, P).

Jointly distributed random variables X & Y, are set to be "equal", $(X = Y)$, when the probability $P\{X = Y\} = 1$. Furthermore, "X" is distributed as Y $(X \sim Y)$, when they possess the same cumulative density function.

Remark: Jointly distributed random variables with the same distribution may not be equal.

e.g. let X be our coin toss Random Variable, as previously defined, & let random variable, Y, be defined, s.t. $Y(T)=1$. & $Y(H)=0$, Then we have $X \sim Y$, but $X \neq Y$.

Definition: A "Random Vector", $\vec{X} = (X_1, X_2, \cdots X_n)$, is a mapping from some Sample space S into $\mathbb{R}^n$, s.t. all the components, X_i, are jointly distributed, & the joint distribution of $\vec{X}$ is given by

$$F_{\vec{X}}(\vec{x}) = P\{X_1 \leq x_1, X_2 \leq x_2, \ldots X_n \leq x_n\}$$

$$\vec{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$$

The components, X_i, are said to be "independent", if the joint distribution function of $\vec{X}$ is given by $F_{\vec{X}}(\vec{x}) = \prod_i F_{X_i}(x_i)$

Definition: A random vector, $\vec{X}$, is "discrete" if there exist countable sets, $\{\vec{x}_i\} \subset \mathbb{R}^n$, and probabilities $\{P_i\} \subset \mathbb{R}_+$, for which

$$P_i = P\{\vec{X} = \vec{x}_i\} > 0, \text{ for all } i,$$

$$\& \sum_i P_i = 1$$

The "joint probability mass function" for $\vec{X}$ is then given by

$$P_{\vec{X}}(\vec{x}) = \begin{cases} P_i, & \text{if } \vec{x} = \vec{x}_i, \ i = 1, 2, \ldots \\ 0, & \text{otherwise} \end{cases}$$

and

$$F_{\vec{X}}(\vec{x}) = \int_{-\infty}^{x_1}\int_{-\infty}^{x_2} \cdots \int_{-\infty}^{x_n} \Big(\sum_i P_i \, \delta(\vec{\mu} - \vec{x})\Big) d\mu_1 d\mu_2 \cdots d\mu_n$$

Definition Random vector, $\vec{X}$, is continuous with "joint probability density function, $P_{\vec{X}}$, if

$$F_{\vec{X}}(\vec{x}) = \int_{-\infty}^{x_1}\int_{-\infty}^{x_2} \cdots \int_{-\infty}^{x_n} P_{\vec{X}}(\vec{\mu})\, d\mu_1\, d\mu_2 \cdots d\mu_n$$

In either the discrete, or the continuous case, if the components, X_i, are independent, then

$$P_{\vec{X}}(\vec{x}) = \prod_{i=1}^{n} P_{X_i}(x_i).$$

where P_{X_i} denotes the Probability density mass function for X_i.

Definition: The mean, or expected value, of a random vector, $\vec{x} = (x_1, x_2, \dots, x_n)$ is the n-vector, $\mathbb{E}(\vec{X})$, having components,

$$[\mathbb{E}(\vec{X})]_i = \mathbb{E}(x_i), \quad i = 1, 2, \dots, n$$

The "Covariance" of $\vec{X}$, is the $n \times n$ matrix, $\mathrm{Cov}(\vec{X}) \in \mathbb{R}^{n\times n}$ (symmetric & positive semi-definite), with components

$$[\mathrm{Cov}(\vec{X})]_{ij} = \mathbb{E}((x_i - \mu_i)(x_j - \mu_j)) \quad 1 \le i, j \le n,$$

where $\mu_i = \mathbb{E}(X_i)$.

Example A continuous random vector, $\vec{X}$, has "Gaussian" or "normal" distribution, if its joint Probability density function has the form:

$$P_{\vec{X}}(\vec{x}; \vec{\mu}, \underline{\underline{C}}) = \frac{1}{\sqrt{(2\pi)^n \det(\underline{\underline{\mathrm{Cov}}})}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu})_i^T \underline{\underline{C}}^{-1}(\vec{x} - \vec{\mu})_i\right)$$

where $\vec{x}, \vec{\mu} \in \mathbb{R}^n$,

& $\underline{\underline{C}} \in \mathbb{R}^{n\times n}$ is symmetric positive semi-definite

The mean is $\mathbb{E}(\vec{X}) = \vec{\mu}$ &

$\mathrm{Cov}(\vec{X}) = \underline{\underline{C}}$, thus we say

$$\vec{X} \sim \mathcal{N}(\vec{\mu}, \underline{\underline{C}})$$

We refer to $\vec{\mu}$ & $\underline{\underline{C}}$ as the parameters of the probability model, described by our n- dimensional Gaussian.