INVERSE PROBLEMS TUTORIAL

INVERSE PROBLEM METHODOLOGY
IN COMPLEX STOCHASTIC SYSTEMS
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STATISTICAL and APPLIED MATHEMATICAL SCIENCES INSTITUTE (SAMSI)

H. T. BANKS

N. C. STATE UNIVERSITY

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Concepts for inverse problems/parameter estimation problems illustrated by ***examples***—Involves both ***deterministic*** and ***probabilistic/stochastic/statistical*** analysis

Includes:

- ***Identifiability***
- ***Ill-posedness***
- ***Stability***
- ***Regularization***
- ***Approximation***
- ***Reduced order modeling {Proper Orthogonal Decomposition(POD)/Principal Component Analysis(PCA)}***

SOME GENERAL REFERENCES:

JOURNALS:

***Inverse Problems*, Institute of Physics Pub. ,(18 Vol thru 2002)**

***J. Inverse and Ill-Posed Problems*, VSP, (9 Vol thru 2001)**

SIAM (J.Control and J.Appl.Math)

BOOKS:

1. G.Anger, *Inverse Problems in Differential Equations*, **Plenum ,N.Y.,1990.**

2. H.T.Banks and K.Kunisch, *Estimation Techniques for Distributed Parameter Systems,* **Birkhauser,Boston,1989.**

3. H.T.Banks,M.W.Buksas,and T.Lin, *Electromagnetic Material Interrogation Using Conductive Interfaces and Acoustic Wavefronts,* **SIAM FR 21,Philadelphia,2002.**

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7. C.W.Groetsch, *Inverse Problems in the Mathematical Sciences*, **Vieweg, Braunschweig,1993.**

8. C.W.Groetsch, *The Theory of Tikhonov Regularization for Fredholm Equations of the First Kind*, **Pitman,London,1984.**

9. B.Hoffman, *Regularization for Applied Inverse and Ill-posed Problems*,**Teubner,Leipzig,1986.**

10. A.N.Tikhonov and V.Y.Arsenin, *Solutions of Ill-posed Problems*, **Winston and Sons,Washington,1977.**

11. C.R.Vogel, *Computational Methods for Inverse Problems*, **SIAM FR23, Philadelphia,2002**

FORWARD PROBLEM
vs.
INVERSE PROBLEM

Parameter dependent dynamical system:

$$\frac{dz}{dt} = g(t, z, \theta), \qquad z(t_0) = z_0, \; g \text{ known}, \; \theta \in \Theta$$

$$z(t) \in R^K, \; \textit{i.e.}, \; z(t) \textit{ is a vector}$$

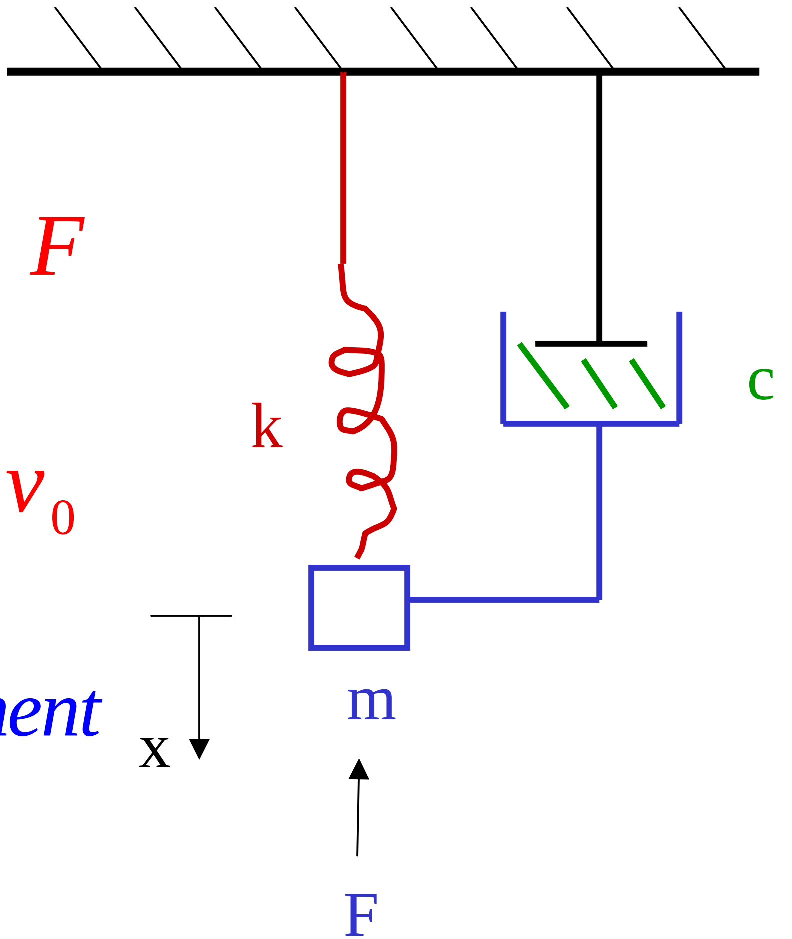
$$\textit{Forward}: \; \textit{Given } \theta, z_0, \textit{ find } z(t) \textit{ for } t \geq t_0$$

$$\textit{Inverse}: \; \textit{Given } z(t) \textit{ for } t \geq t_0, \textit{ find } \theta \in \Theta$$

Mass-spring-dashpot system

$$m\frac{d^2x}{dt^2}+c\frac{dx}{dt}+kx=F$$

$$x(0)=x_0 \qquad \frac{dx}{dt}(0)=v_0$$



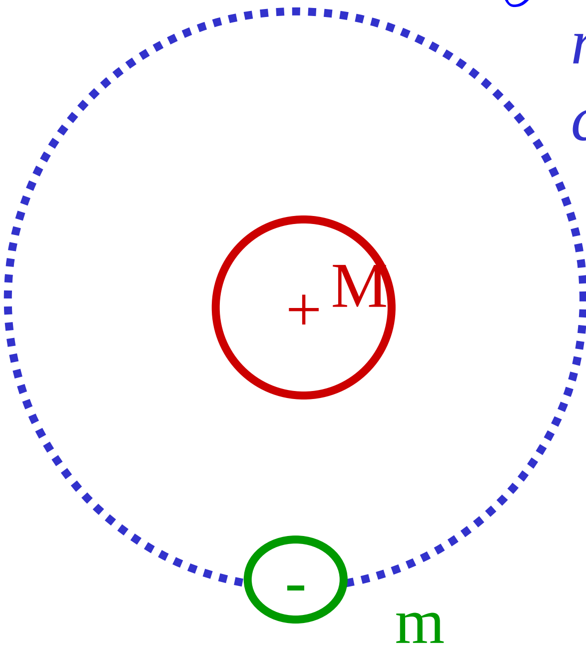
x = equilibrium displacement of mass m

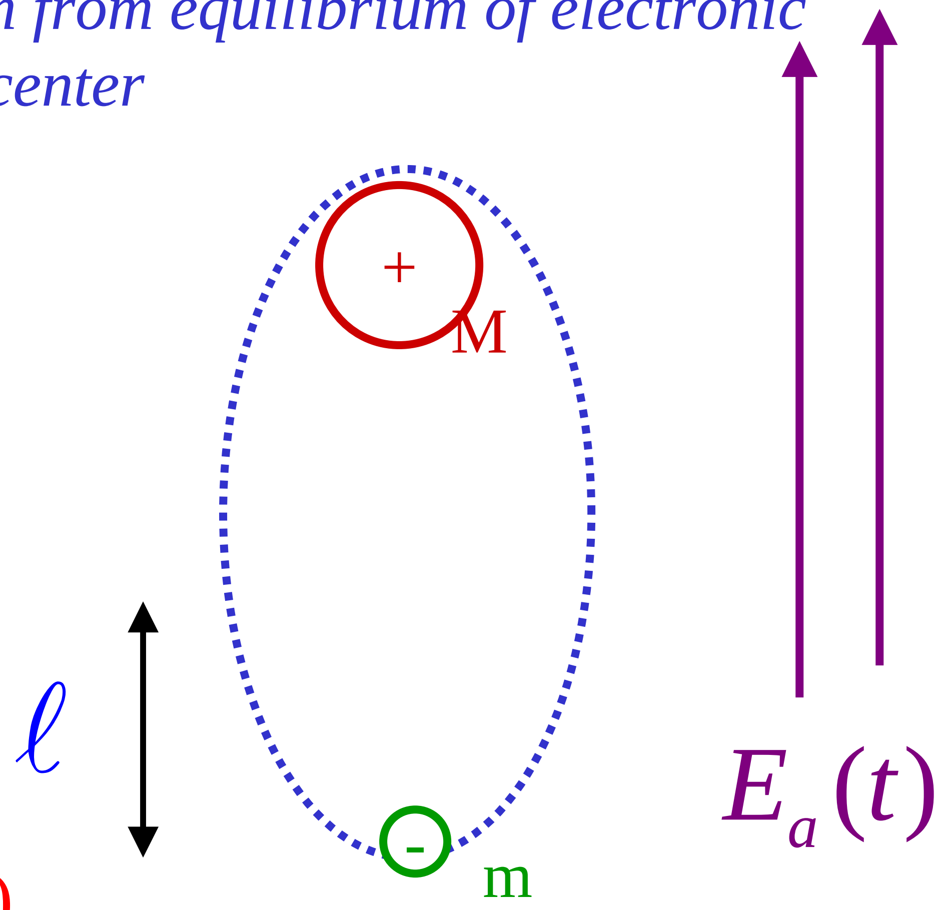
$Forward: \ Given\ m, c, k, F, x_0, v_0,\ find\ x(t)\ for\ t > t_0$

$Inverse: \ Given\ x(t)\ for\ t \geq t_0,\ v_0,\ and\ F,\ find\ m, c, and\ k$

Electronic Polarization—electronic cloud displacement

ℓ = displacement of negative charge of mass m from equilibrium of electronic cloud center





$$m\frac{d^2\ell}{dt^2}+c\frac{d\ell}{dt}+k\ell=QE_a(t)$$

Usually are not given observations of all of system state z(t):
Example(mass-spring-dashpot system):
First, rewrite as first order vector system:

$$z(t) = \begin{pmatrix} x(t) \\ \dfrac{dx(t)}{dt} \end{pmatrix}, \quad \frac{dz(t)}{dt} = A(\theta) z(t) + F(t), \; z_0 = \begin{pmatrix} x_0 \\ v_0 \end{pmatrix}$$

$$A(\theta) = \begin{pmatrix} 0 & 1 \\ -\dfrac{k}{m} & -\dfrac{c}{m} \end{pmatrix} \quad F(t) = \begin{pmatrix} 0 \\ \dfrac{F(t)}{m} \end{pmatrix} \quad \theta = \left(\frac{k}{m}, \frac{c}{m} \right)$$

$$\textit{Observations}: \; f(t,\theta) = \mathsf{C}\; z(t,\theta)$$

$$\textit{Laser vibrometer}: \; f(t,\theta) = v(t) = \frac{dx(t)}{dt}$$

$$\textit{Observation operator}: \; \mathsf{C} = (0 \quad 1)$$

$$\textit{Proximity probe}: \; f(t,\theta) = x(t)$$

$$\textit{Observation operator}: \; \mathsf{C} = (1 \quad 0)$$

More likely, discrete (finite number) observations:

$$\left\{ \tilde{y}_j \right\}_{j=1}^{n} \quad \textit{where } \tilde{y}_j \approx f(t_j,\theta)$$

Can formulate as least–squares fit of

model *to* observations:

$$J(\theta)=\sum_{j=1}^{n}\left|\tilde{y}_j - f(t_j,\theta)\right|^2$$

where f is the model solution(response) or that part of the solution that we can "observe" or that we care about in design!

"Model driven" vs. "data driven" inverse problems

$$Model\ driven:\ \ \tilde{y}_j = f(t_j, \theta)$$

$$Data\ driven:\ \ \tilde{y}_j = f(t_j, \theta) + \varepsilon_j,\ \ \varepsilon_j\ is\ error$$

$$(Depending\ on\ the\ error,\ may\ need\ to\ introduce\ variability\ into\ the\ modeling\ and\ analysis)$$

$Model\ driven:\ \tilde{y}_j = f(t_j, \theta)$

i) System Design problems

a) design of spring / shock system (automotive, "smart" truck seats)

b) design of thermally conductive epoxies for use in computer motherboards

ii) Nondestructive Evaluation (NDE) *problems*

a) thermal interrogation of conductive structures

b) eddy current – based electromagnetic damage detection

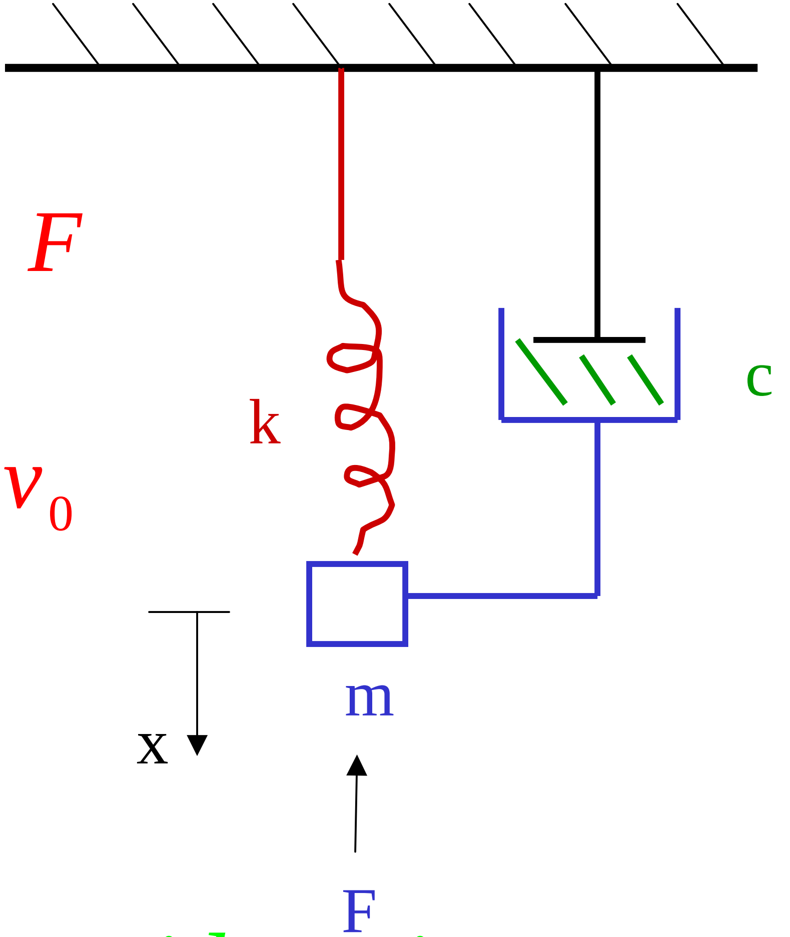
Design of spring/shock system

(automotive, "smart" truck seats)

Mass-spring-dashpot system

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = F$$

$$x(0) = x_0 \qquad \frac{dx}{dt}(0) = v_0$$



$$\left\{\begin{array}{l} Choose\ \theta = (k,c)\ to\ provide\ a\ given\ \ response \\ x(t)\ for\ a\ \text{"}load\text{"}\ m\ and\ perturbation\ F(t) \end{array}\right\}$$

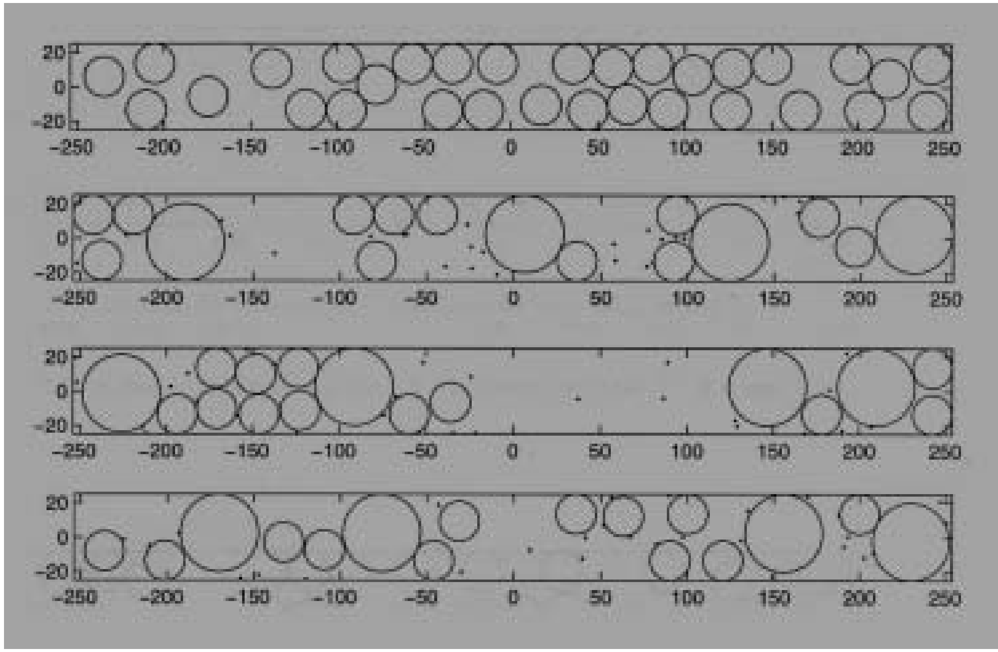
DESIGN OF THERMALLY CONDUCTIVE COMPOSITE ADHESIVES

GOALS

Design and analysis of thermally conductive composite adhesives (epoxies and gels filled with highly conductive particles such as aluminum, diamond dust, and carbon)

POTENTIAL AND SIGNIFICANCE

Development of enhanced thermally conductive adhesives for microelectronic devices,automotive and aeronautical components



Determine $\rho, c_p,$ *and* k *(all spatially varying) in*

$$\rho(\vec{x})c_p(\vec{x})\frac{\partial u(t,\vec{x})}{\partial t} = \nabla(k(\vec{x})\nabla u(t,\vec{x}))$$

for a desired temperature u *or flux* $\dfrac{\partial u}{\partial n} = \nabla u \bullet \vec{n}$

on the boundary

References:

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2) **K.L.Bihari, *Analysis of Thermal Conductivity in Composite Adhesives*, Ph.D. Thesis, NCSU, August, 2001.**

3) **H.T.Banks and K.L.Bihari, Analysis of thermal conductivity in composite adhesives, CRSC-TR01-20, NCSU, August, 2001; Numerical Functional Analysis and Optimization, Dec.,2002, to appear.**

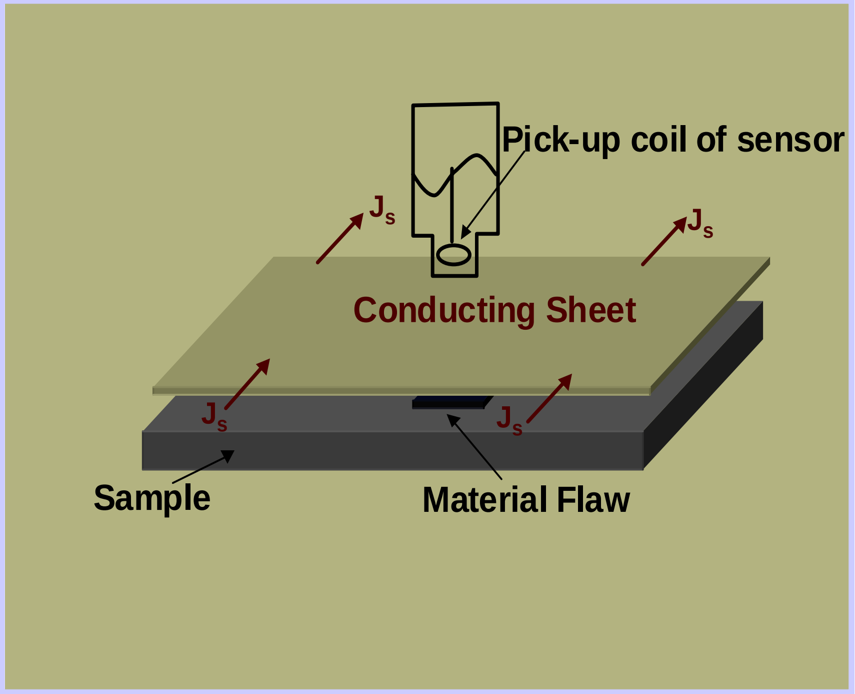
DAMAGE DETECTION USING EDDY CURRENT TECHNIQUES

GOALS

Develop fast on-line computational methods for use with highly sensitive magnetic flux sensors in detection of subsurface damages

POTENTIAL AND SIGNIFICANCE

Development of portable, real time scanning devices for damage detection in conductive materials. Potential for fast scanners for nondestructive evaluation in aging aircraft, spacecraft and other structures



Using measurements of the magnetic vector potential $\mathbf{A}$, *determine any voids in the material (characterized by* $\sigma = 0$) *where*

$$\nabla \times \left(\frac{1}{\mu(x,y)} \nabla \times \mathbf{A}(x,y) \right) = \left(\sigma(x,y) + i\omega\varepsilon(x,y) \right) \left(-i\omega \mathbf{A}(x,y) - \nabla \phi \right) \quad for \ (x,y) \in \Omega,$$

$$I_{cs} = \int_{cs} \left(\sigma(x,y) + i\omega\varepsilon(x,y) \right) \left(-i\omega \mathbf{A}(x,y) - \nabla \phi \right) \cdot \mathbf{n} da \quad for \ (x,y) \in cs$$

References:

1) **H.T.Banks,M.L.Joyner,B.Wincheski,and W.P.Winfree, Evaluation of material integrity using reduced order computational methodology, CRSC-TR99-30, NCSU, August, 1999.**

2) **H.T.Banks,M.L.Joyner,B.Wincheski,and W.P.Winfree, Nondestructive evaluation using a reduced-order computational methodology, ICASE Tech Rep 2000-10, NASA LaRC, March 2000; Inverse Problems 16(2000),929-945.**

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4) **H.T.Banks,M.L.Joyner,B.Wincheski,and W.P.Winfree, Electromagnetic interrogation techniques for damage detection,CRSC-TR01-15,NCSU, June,2001; Proceedings ENDE0 (Kobe, Japan, May,2001), to appear.**

5) **H.T.Banks,M.L.Joyner,B.Wincheski,and W.P.Winfree, Real time computational algorithms for eddy current based damage detection, CRSC-TR01-16,NCSU,June,2001; Inverse Problems, to appear.**

6) **M.L.Joyner, *An Application of a Reduced Order Computational Methodolgy for Eddy Current Based Nondestructive Evaluation Techniques*, Ph.D. Thesis, NCSU, June, 2001.**

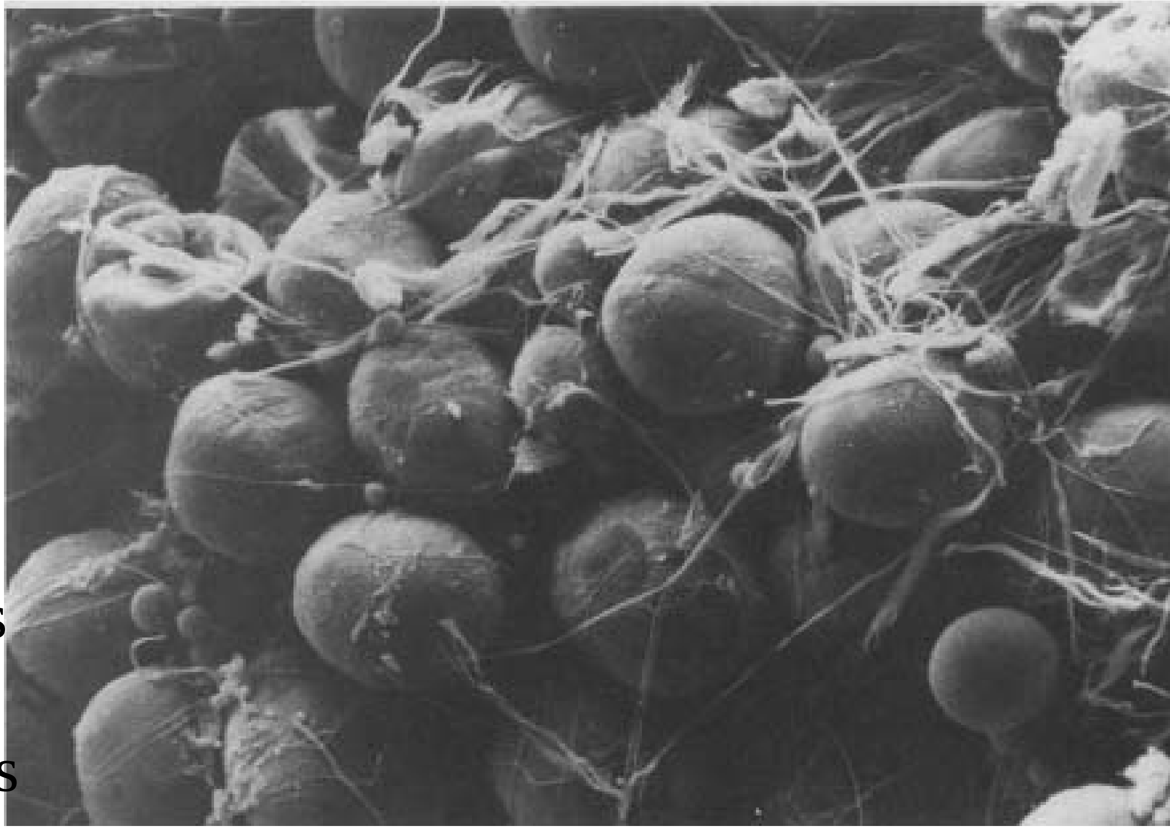
$\textit{Data driven}: \ \tilde{y}_j = f(t_j, \theta) + \varepsilon_j, \ \ \varepsilon_j \textit{ is error}$

Many (most!) of examples lead to the introduction of *variability* into both the modeling and the analysis!!

i) Physiologically Based Pharmacokinetic (PBPK) modeling in toxicokinetics

ii) Modeling of HIV pathogenesis

PBPK Models for TCE in Fat Cells



Millions of cells with varying size, residence time, vasculature, geometry: "Axial-dispersion" type adipose tissue compartments to embody uncertain physiological heterogeneities in single organism (rat) = ***intra-individual variability***

Inter-individual variability treated with parameters (including dispersion parameters) as ***random variables*** –estimate ***distributions*** from aggregate data (multiple rat data) which also contains uncertainty (noise)

Whole-body system of equations

$$V_v \frac{dC_v(t)}{dt} = Q_f C_B(t, \pi - \varepsilon_2) + \frac{Q_{br}}{P_{br}} C_{br}(t) + \frac{Q_k}{P_k} C_k(t) + \frac{Q_l}{P_l} C_l(t) + \frac{Q_m}{P_m} C_m(t) + \frac{Q_t}{P_t} C_t(t) - Q_c C_v(t)$$

$$C_a(t) = \left(Q_c C_v(t) + Q_p C_c(t)\right) \Big/ \left(Q_c + Q_p / P_b\right)$$

$$V_{br} \frac{dC_{br}(t)}{dt} = Q_{br}\left(C_a(t) - C_{br}(t)/P_{br}\right)$$

$$V_B \frac{\partial C_B}{\partial \phi} = \frac{V_B}{r_2 \sin\phi} \frac{\partial}{\partial \phi}\left[\sin\phi \left(\frac{D_B}{r_2} \frac{\partial C_B}{\partial \phi} - v C_B\right)\right] + \lambda_I \mu_{BI}\left(f_I C_I(\theta_0) - f_B C_B\right) + \lambda_A \mu_{BA}\left(f_A C_A(\theta_0) - f_B C_B\right)$$

$$V_I \frac{\partial C_I}{\partial t} = \frac{V_I D_I}{r_1^2}\left[\frac{1}{\sin^2\phi} \frac{\partial^2 C_I}{\partial \theta^2} + \frac{1}{\sin\phi} \frac{\partial}{\partial \phi}\left(\sin\phi \frac{\partial C_I}{\partial \phi}\right)\right] + \delta_{\theta_0}(\theta)\chi_B(\phi)\lambda_I \mu_{BI}\left(f_B C_B - f_I C_I\right) + \mu_{IA}\left(f_A C_A - f_I C_I\right)$$

$$V_A \frac{\partial C_A}{\partial t} = \frac{V_A D_A}{r_0^2}\left[\frac{1}{\sin^2\phi} \frac{\partial^2 C_A}{\partial \theta^2} + \frac{1}{\sin\phi} \frac{\partial}{\partial \phi}\left(\sin\phi \frac{\partial C_A}{\partial \phi}\right)\right] + \delta_{\theta_0}(\theta)\chi_B(\phi)\lambda_A \mu_{BA}\left(f_B C_B - f_A C_A\right) + \mu_{IA}\left(f_I C_I - f_A C_A\right)$$

$$V_k \frac{dC_k(t)}{dt} = Q_k\left(C_a(t) - C_k(t)/P_k\right)$$

$$V_l \frac{dC_l(t)}{dt} = Q_l\left(C_a(t) - \frac{C_l(t)}{P_l}\right) - \left(v_{\max} \frac{C_l(t)}{P_l}\right) \Big/ \left(k_M + \frac{C_l(t)}{P_l}\right)$$

$$V_m \frac{dC_m(t)}{dt} = Q_m\left(C_a(t) - C_m(t)/P_m\right)$$

$$V_t \frac{dC_t(t)}{dt} = Q_t\left(C_a(t) - C_t(t)/P_t\right)$$

Plus boundary conditions
and initial conditions

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2)H.T.Banks and L.K.Potter,Well-posedness results for a class of toxicokinetic models,CRSR-TR01-18,NCSU,July,2001; Discrete and Continuous Dynamical Systems,submitted

3)L.K.Potter,*Physiologically based pharmacokinetic models for the systemic transport of Trichloroethylene*, Ph.D. Thesis,NCSU, August, 2001

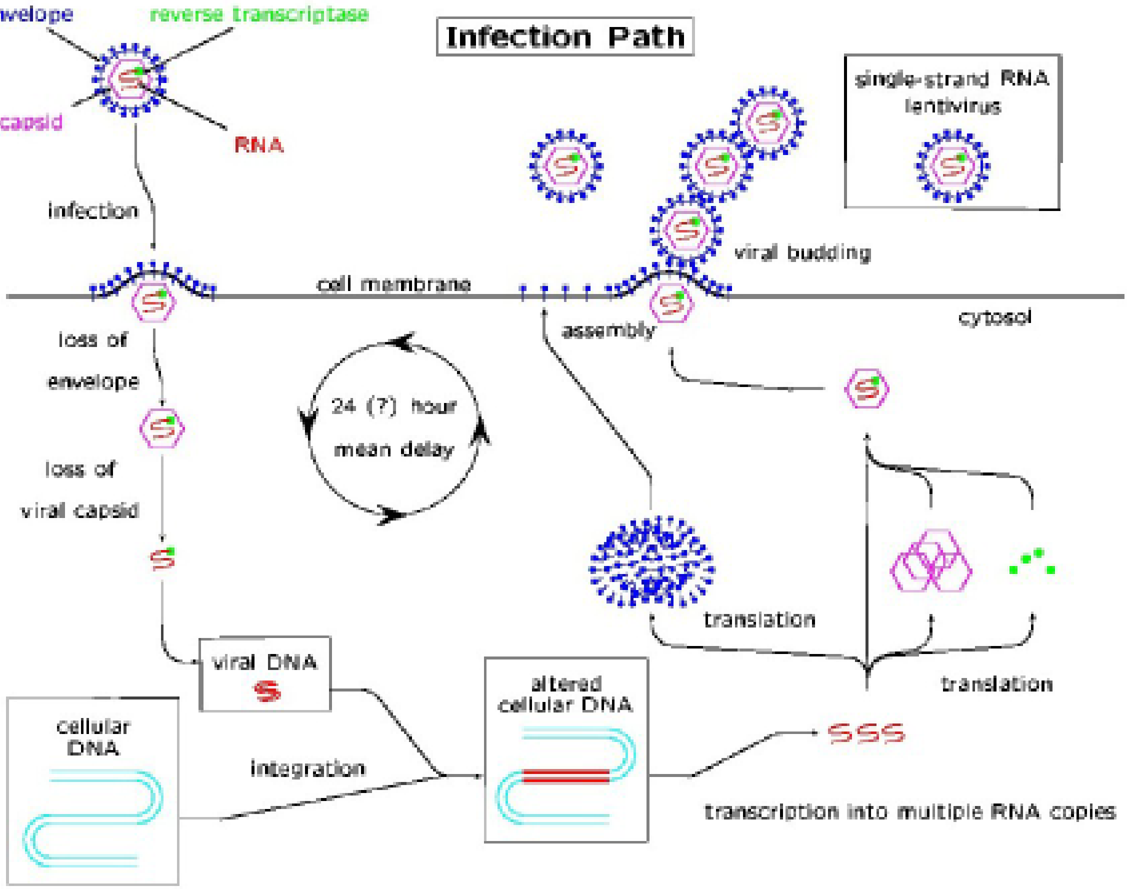
4)H.T.Banks and L.K. Potter, Model predictions and comparisions for three Toxicokinetic models for the systemic transport of TCE,CRSC-TR01-23,NCSU, August,2001; Mathematical and Computer Modeling 35(2002), 1007-1032

5)H.T.Banks and L.K.Potter, Probabilistic methods for addressing uncertainty and variability in biological models: Application to a toxicokinetic model, CRSC-TR02-27,NCSU,Sept.2002; Math. Biosciences, submitted.

MODELING OF HIV PATHOGENESIS

GOALS

DEVELOPMENT OF DYNAMIC MODELS INVOLVING INTRA- AND INTER-INDIVIDUAL VARIABILITY TO AID IN UNDERSTANDING OF FUNDAMENTAL MECHANISMS OF INFECTION AND SPREAD OF DISEASE-AGGREGATE DATA ACROSS POPULATIONS



POTENTIAL AND SIGNIFICANCE

POPULATION LEVEL ESTIMATION OF SPREAD RATES AND EFFICACY IN TREATMENT PROGRAMS FOR EXPOSURE

Involves systems of equations of the form (generally nonlinear)

$$\frac{dV}{dt} = -cV(t) + n_a A(t-\tau) + n_c C(t) - n_{vt} V(t) T(t)$$

where τ is a production delay (distributed across the population of cells). That is, one should write

$$\frac{dV}{dt} = -cV(t) + n_a \int_0^{\infty} A(t-\tau) k(\tau) d\tau + n_c C(t) - n_{vt} V(t) T(t)$$

where **k is a probability density to be estimated from aggregate data.**

Even if **k** is given, these systems are nontrivial to simulate—require development of fundamental techniques.

HIV Model:

$$\dot{V}(t) = -cV(t) + n_A \int_0^r A(t-\tau)\,d\pi_1(\tau) + n_C C(t) - p(V,T)$$

$$\dot{A}(t) = (r_v - \delta_A - \delta X(t))A(t) - \gamma \int_0^r A(t-\tau)\,d\pi_2(\tau) + p(V,T)$$

$$\dot{C}(t) = (r_v - \delta_C - \delta X(t))C(t) + \gamma \int_0^r A(t-\tau)\,d\pi_2(\tau)$$

$$\dot{T}(t) = (r_u - \delta_u - \delta X(t))T(t) - p(V,T) + S$$

where $C(t) = \mathrm{E}_2\{C(t;\tau)\} = \int_0^r C(t;\tau)\,d\pi_2(\tau)$, $A =$ acute cells

$V(t) = V_A(t) + V_C(t),\ V_A(t) = \mathrm{E}_1\{V_A(t;\tau)\} = \int_0^r V_A(t;\tau)\,d\pi_1(\tau)$

$\pi_1 \sim$ delay from acute infection to viral production

$\pi_2 \sim$ delay from acute infection to chronic infection

$T =$ target cells, $X =$ total (infected+uninfected) cells

References:

1) D. Bortz, R. Guy, J. Hood, K. Kirkpatrick, V. Nguyen, and V. Shimanovich, Modeling HIV infection dynamics using delay equations, in 6th CRSC Industrial Math Modeling Workshop for Graduate Students, NCSU(July,2000), CRSC TR00-24, NCSU, Oct, 2000

2) H. T. Banks, D. M. Bortz, and S. E. Holte, Incorporation of variability into the modeling of viral delays in HIV infection dynamics, CRSC-TR01-25, Sept, 2001; Math Biosciences, submitted.

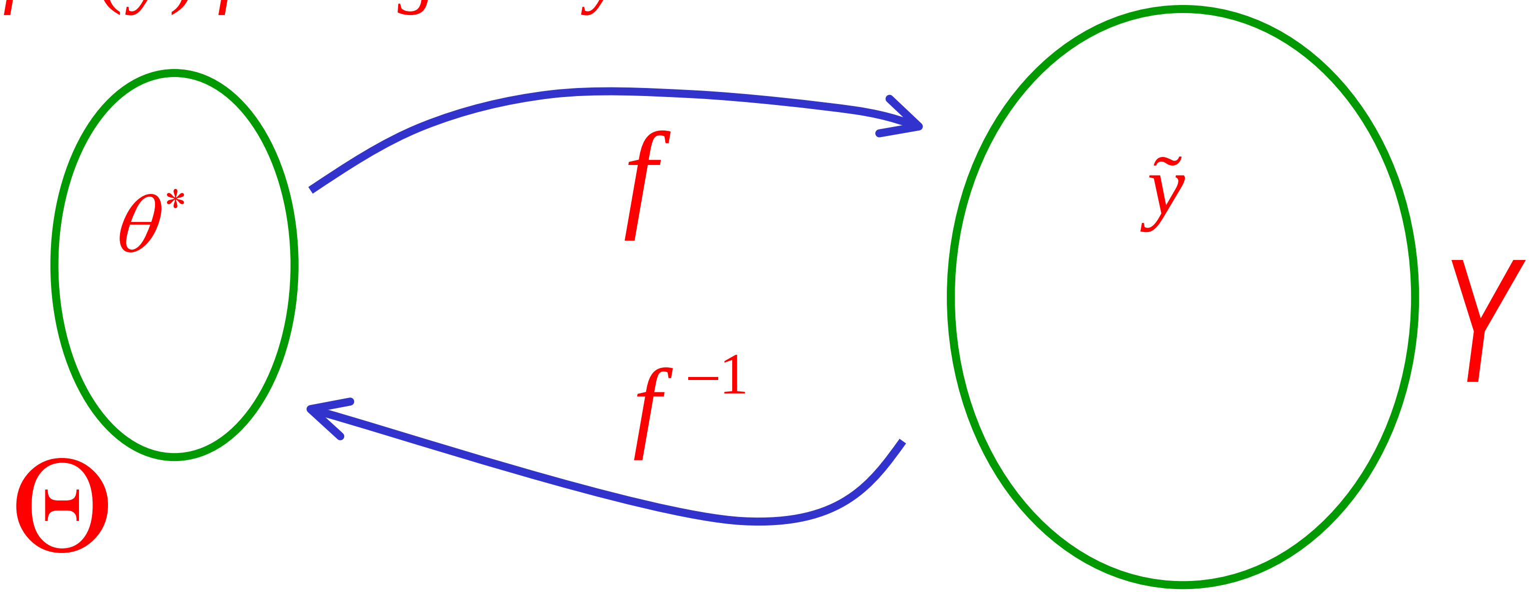
3) H.T.Banks and D.M.Bortz, A parameter sensitivity methodology in the context of HIV delay equation models, CRSC-TR02-24, August, 2002; J. Math. Biology, submitted

4) D.M.Bortz, *Modeling, Analysis,and Estimation of an In Vitro HIV Infection Using Functional Differential Equations*, Ph. D. Thesis, NCSU, August, 2002.

The problems above are (as are most others) notoriously *ill-posed*!! This concept is difficult to explain in the context of the problems outlined above—so we turn to some exceedingly simple examples to illustrate the ideas behind *well-posedness!*   *Simplest case:*

one observation – $\tilde{y}$ *for* $f(\theta)$ *– and need to find preimage*

$\theta^* = f^{-1}(\tilde{y})$ *for a given* $\tilde{y}$



Well-posedness:

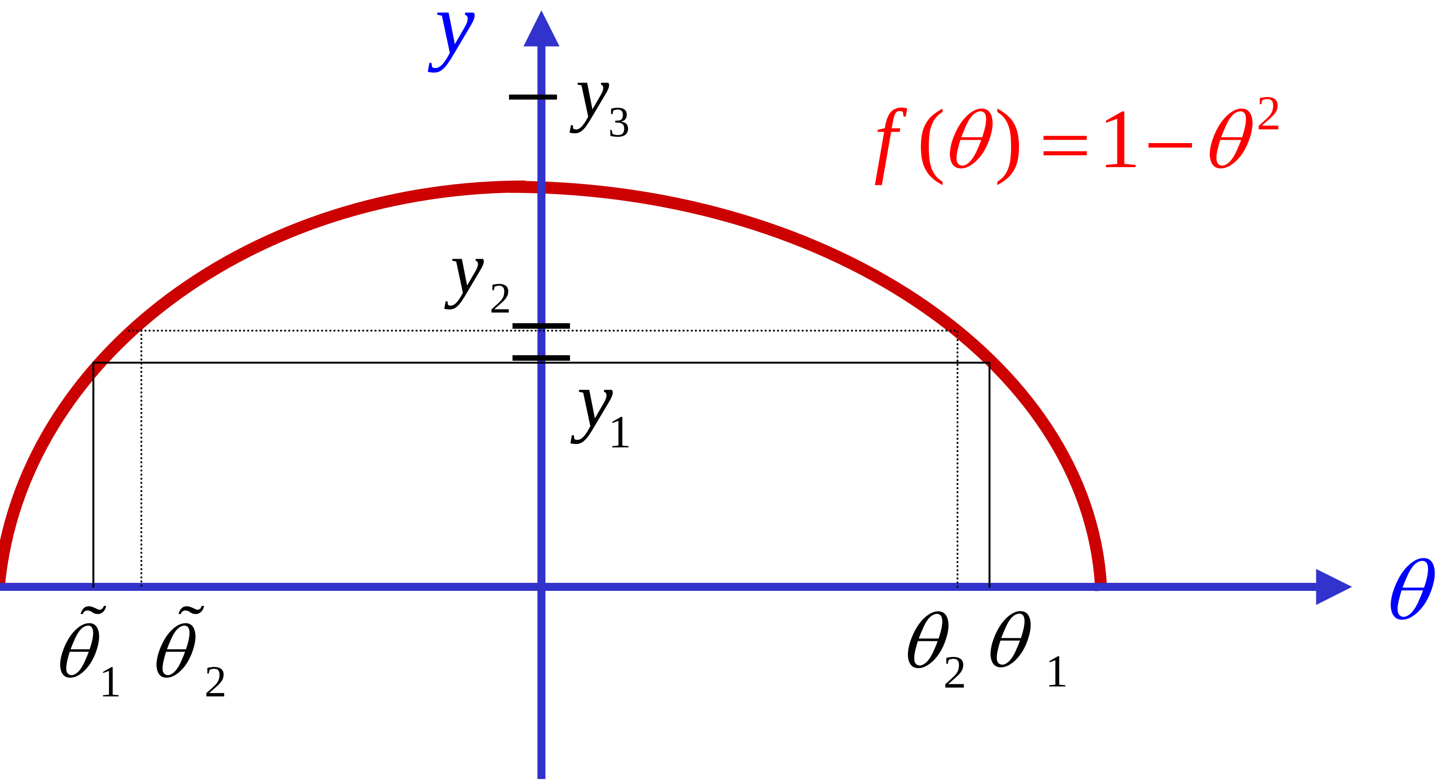
i. Existence

i. Uniqueness

Identifiability

ii. Continuous dependence of solutions on observations

"stability" of inverse problem



Non-existence: No θ_3 such that $f(\theta_3) = y_3$

Non-uniqueness: $y_j = f(\theta_j) = f(\tilde{\theta}_j) \quad j = 1, 2$

Lack of continuity of inverse map:

$$|y_1 - y_2| \ \text{small} \quad \not\Rightarrow \quad \left| f^{-1}(y_1) - f^{-1}(y_2) \right|$$

$$= \left| \theta_1 - \tilde{\theta}_2 \right| \ \text{small}$$

Why is this so important???

Why not just apply a good numerical algorithm for a least squares (for example) fit to try to find the "best" possible solution???? (Seldom expect zero residual!!)

Define $J(\theta) = \left| y_1 - f(\theta) \right|^2$ *for a given* y_1

and then apply a standard iterative method to obtain a solution!!

Iterative methods:

1) *Direct search (simplex, Nelder-Mead,………)*
2) *Gradient based (Newton, steepest descent, conjugate gradient,………)*

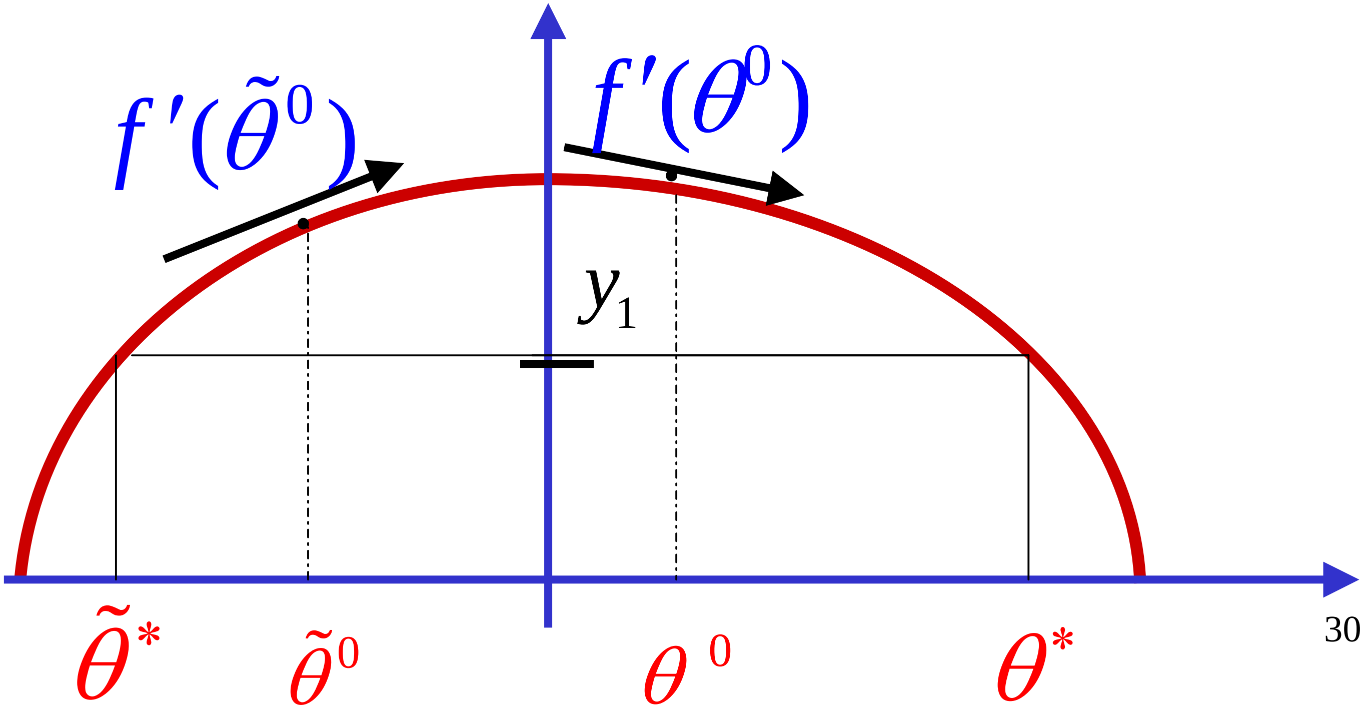
$$e.g., \text{ Newton: } \theta^{k+1} = \theta^{k} - [J'(\theta^{k})]^{-1} J(\theta^{k})$$

$$\theta^{k+1} = \theta^{k} - [J'(\theta^{k})]^{-1} J(\theta^{k})$$

$$For \quad J(\theta) = \left| y_1 - f(\theta) \right|^2 \quad , J'(\theta) = 2(y_1 - f(\theta))(-f'(\theta))$$

$$J'(\theta^0) = 2(-)(- \; -) < 0, \;\; \Rightarrow \theta^1 > \theta^0, \;\; etc.$$

$$J'(\tilde{\theta}^0) = 2(-)(- \; +) > 0, \;\; \Rightarrow \tilde{\theta}^1 < \tilde{\theta}^0, \;\; etc.$$



This behavior is not the fault of steepest descent algorithms, but is a manifestation of the inherent "ill-posedness" of the problem!!

How to fix this is the subject of much research over the past 40 years!! Among topics are:

i) constrained optimization { **explicit(compact constraint sets)**, **implicit(Lagrange multipliers)** }

ii) regularization { **a) Tikhonov regularization(1963) (compactification, convexification)**, **b) regularization by discretization** }

Tikhonov regularization

$$Idea: \quad Problem\ for\ J(\theta) = \left| y_1 - f(\theta) \right|^2\ is\ ill-posed,$$

$$so\ replace\ it\ by\ a\ "near-by"\ problem\ for$$

$$J_\beta(\theta) = \left| y_1 - f(\theta) \right|^2 + \beta \left| \theta - \theta_0 \right|^2$$

$$where\ \beta\ is\ a\ regularization\ parameter\ to\ be$$

$$"appropriately\ chosen"\ !!$$

PRO: When done correctly, provides convexity and compactness in the problem!

CON: Even when done correctly, it changes the problem and solutions to the new problems may not be close to those of original! Moreover, it is not easy to do correctly or even to know if you have done so!!

EXAMPLE:

$f(\theta) = 1 + \alpha \sin(\pi\theta), \qquad \beta \textit{ ranging from } \beta = 0 \textit{ to}$

$100 \textit{ thru values } 0,\ .01,\ \ldots, 1.0,\ \ldots, 10,\ \ldots, 40,\ \ldots, 80,\ 100,$

$\textit{several values of } \alpha,\ \theta_0,\ \textit{and } y_1$

1) $\alpha = 1,\ y_1 = 1.5,\ \ \theta_0 = 0$ (tik)*

2) $\alpha = .5,\ y_1 = .8,\ \ \theta_0 = 0$ (tik1)

3) $\alpha = .5,\ y_1 = 1.6$ ($\textit{not in range of } f$), $\theta_0 = 0$ (tik2)*

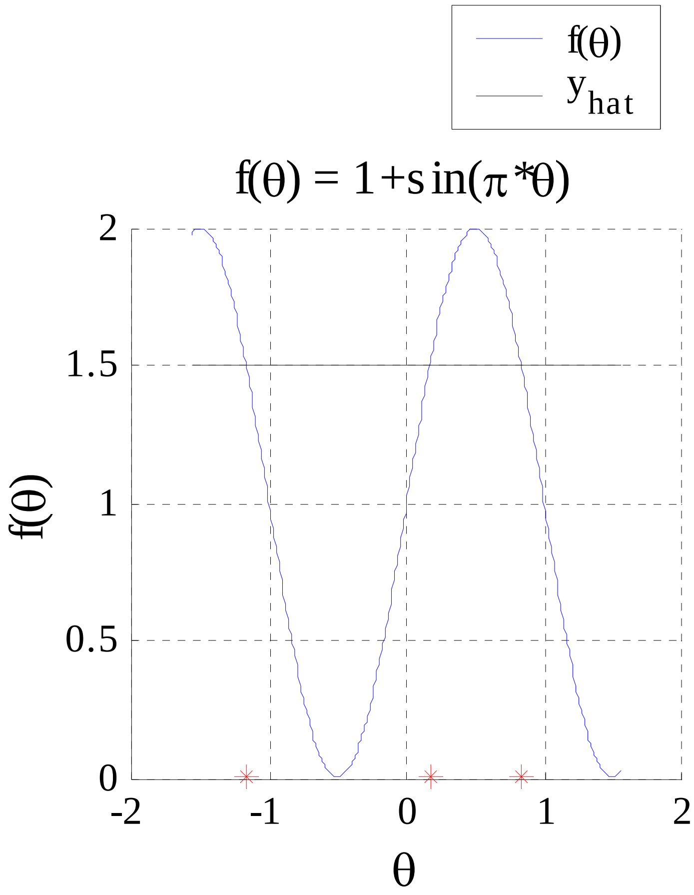
4) $\alpha = 1,\ y_1 = 1.5,\ \ \theta_0 = 1.0$ (tik4)

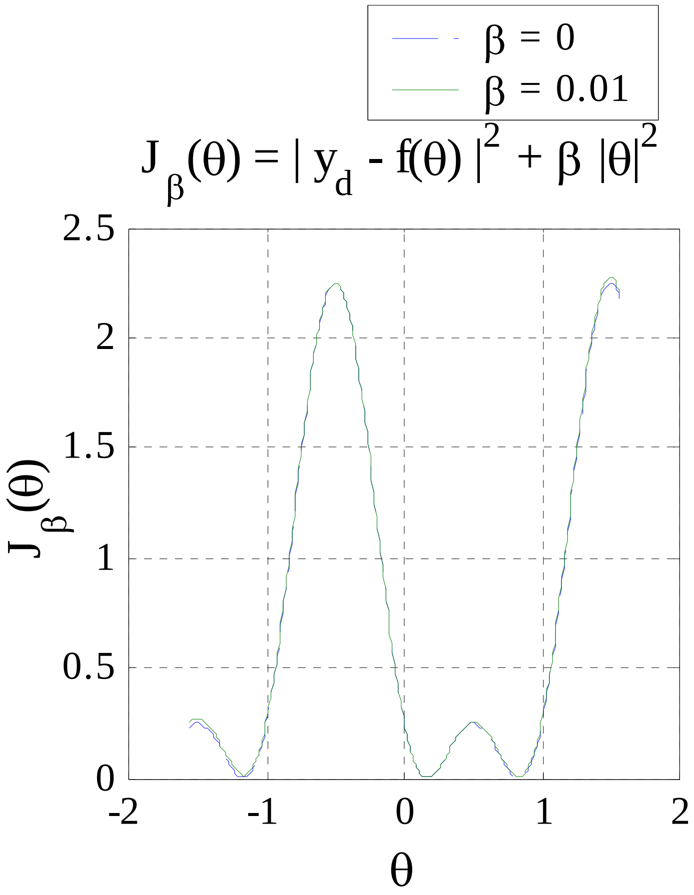
5) $\alpha = 1,\ y_1 = 1.5,\ \ \theta_0 = 1.8$ (tik6)*

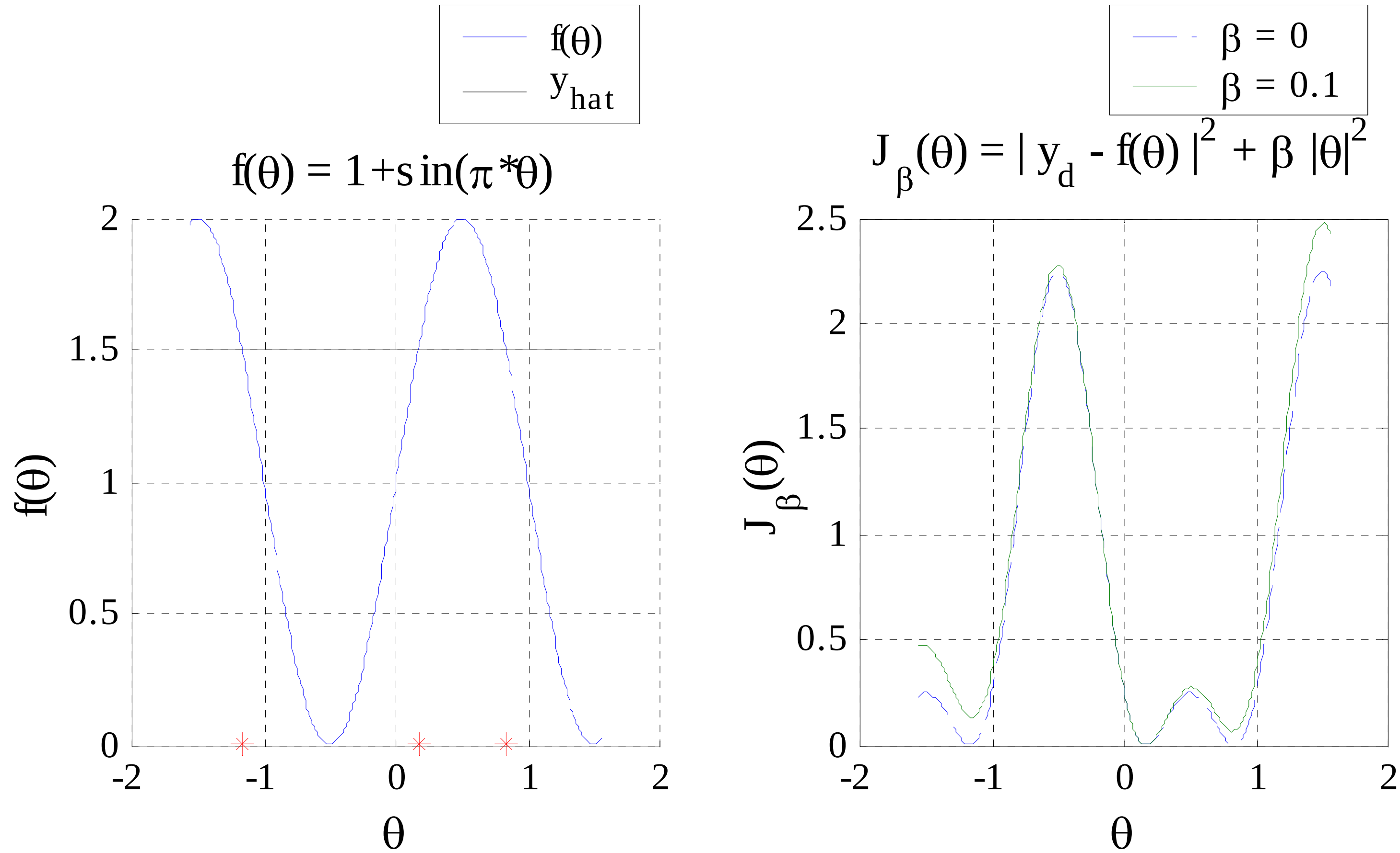
6) $\alpha = 1,\ y_1 = 1.5,\ \ \theta_0 = .5$ (tik7)*

7) $\alpha = 1,\ y_1 = 1.5,\ \ \theta_0 = -.5$ (tik8)*

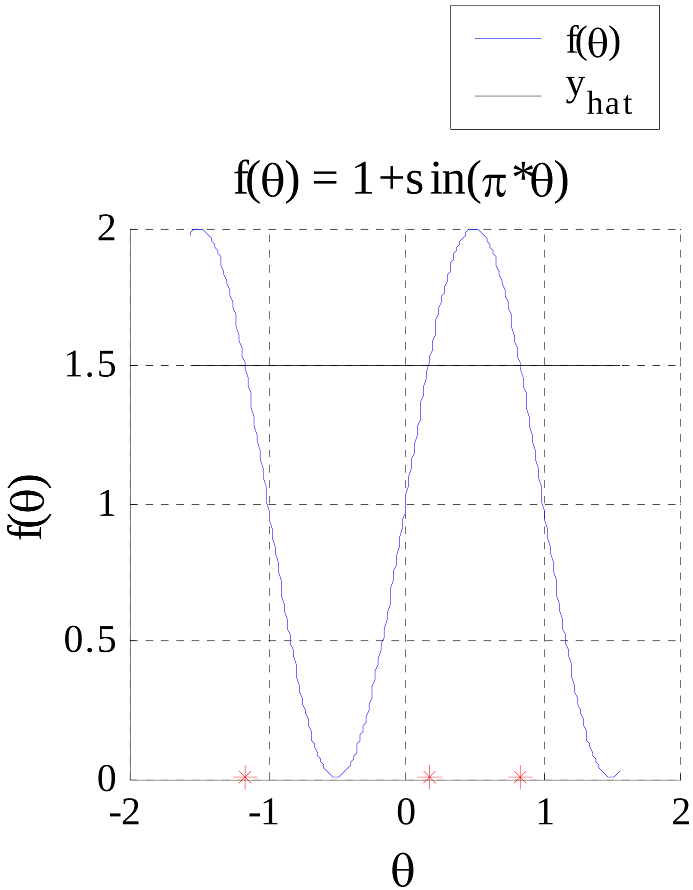
$(alt\,/\,tab)$

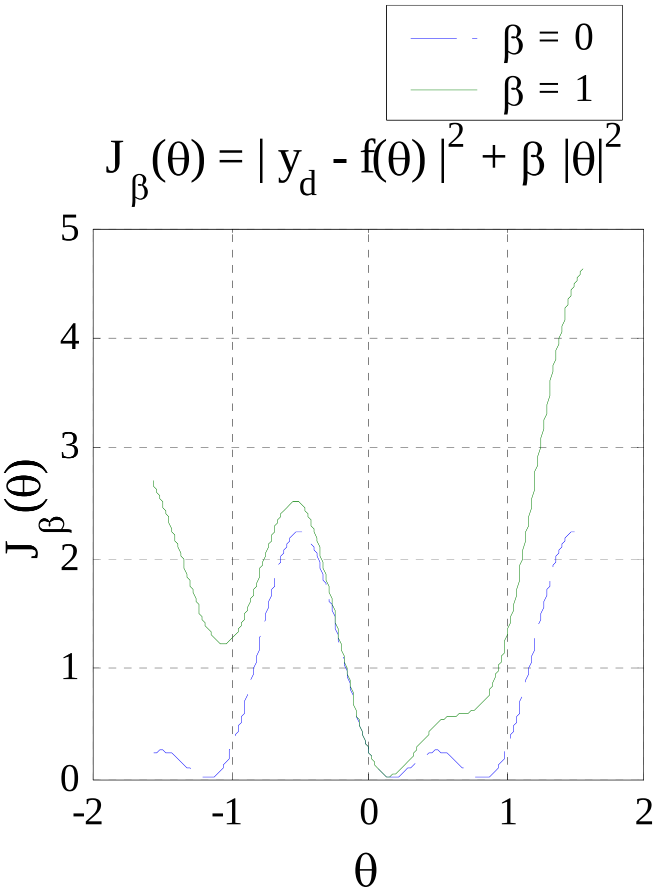

f(θ)
y_hat
f(θ) = 1+sin(π*θ)
2
1.5
1
0.5
0
-2
-1
0
1
2
f(θ)
θ

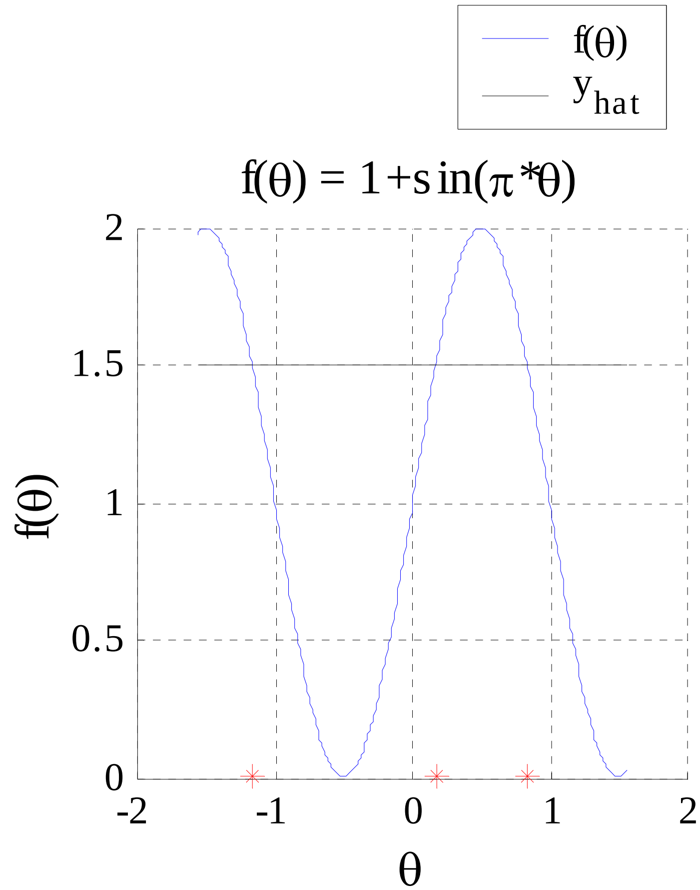

β = 0
β = 0.01
J_β(θ) = | y_d - f(θ) |^2 + β |θ|^2
2.5
2
1.5
1
0.5
0
-2
-1
0
1
2
J_β(θ)
θ



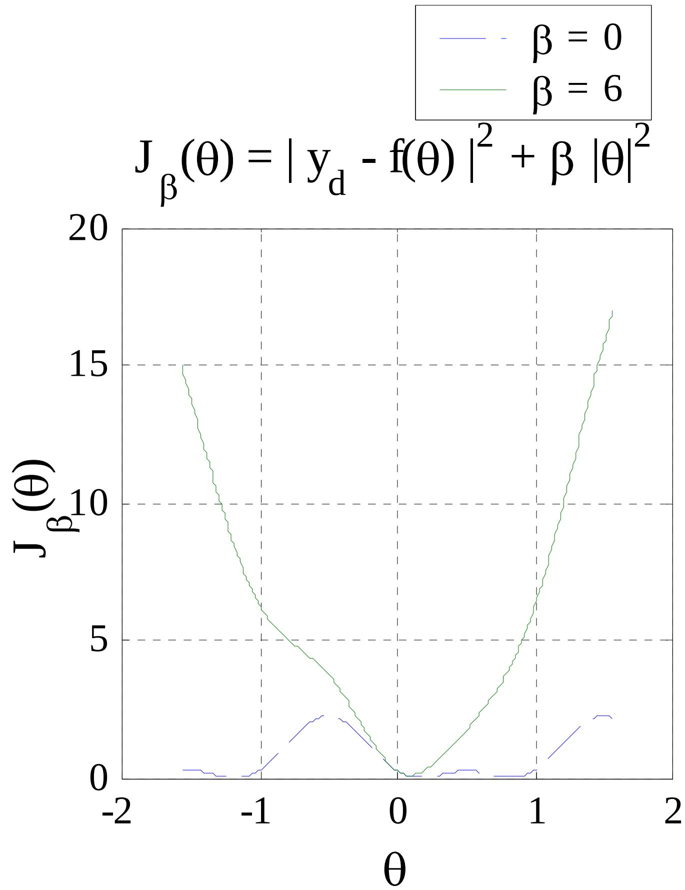
f(θ)
y_hat
f(θ) = 1+sin(π*θ)
f(θ)
θ
2
1.5
1
0.5
0
-2
-1
0
1
2
β = 0
β = 0.1
J_β(θ) = | y_d - f(θ) |^2 + β |θ|^2
J_β(θ)
θ
2.5
2
1.5
1
0.5
0
-2
-1
0
1
2


f(θ)
y_hat
f(θ) = 1+sin(π*θ)
2
1.5
1
0.5
0
-2
-1
0
1
2
f(θ)
θ

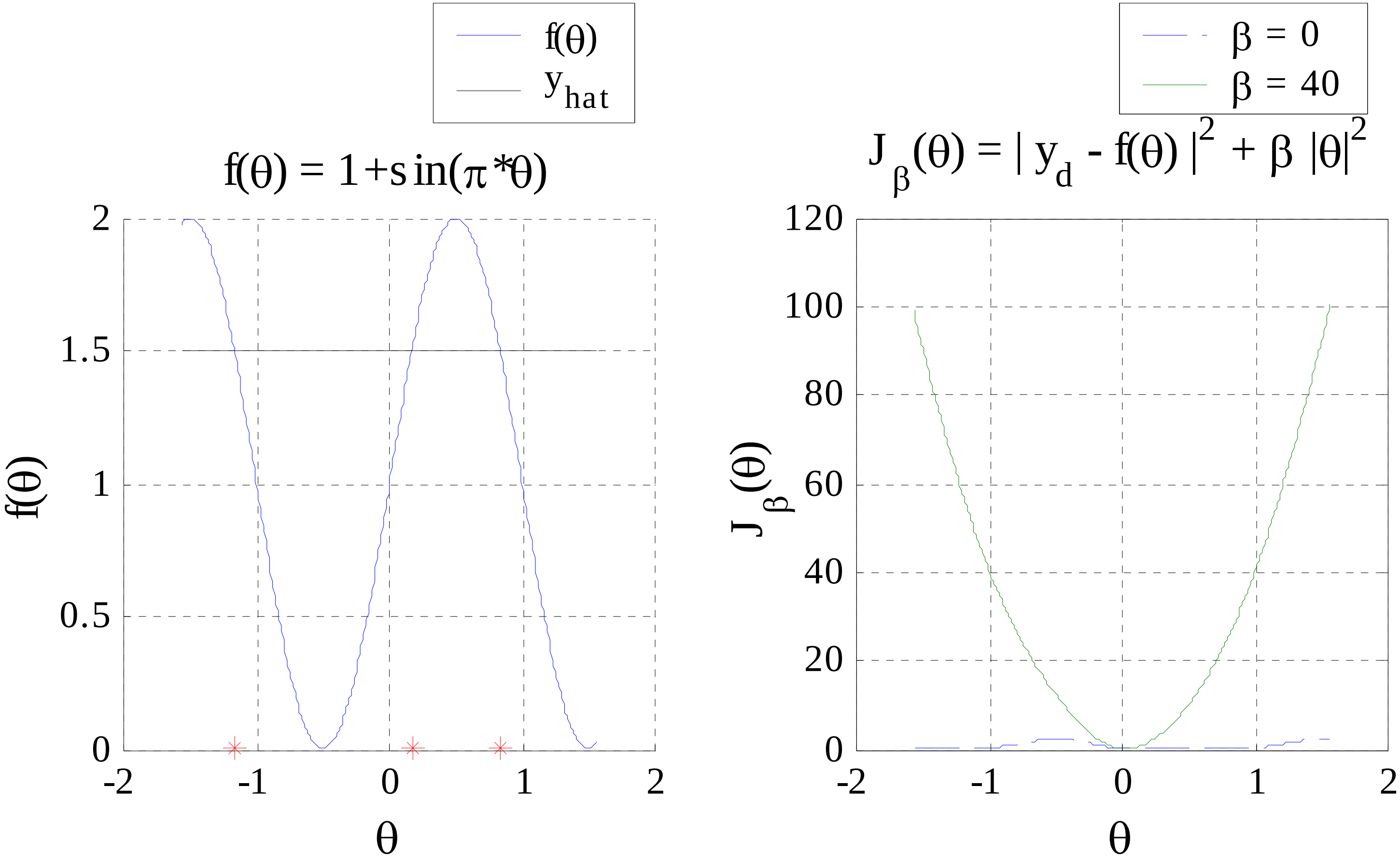

β = 0
β = 1
J_β(θ) = | y_d - f(θ) |^2 + β |θ|^2
5
4
3
2
1
0
-2
-1
0
1
2
J_β(θ)
θ



f(θ)
y_{hat}
$f(\theta) = 1+\sin(\pi*\theta)$
2
1.5
1
0.5
0
-2
-1
0
1
2
f(θ)
θ



$\beta = 0$
$\beta = 6$
$J_\beta(\theta) = | y_d - f(\theta) |^2 + \beta\ |\theta|^2$
20
15
10
5
0
-2
-1
0
1
2
$J_\beta(\theta)$
θ



f(θ)
y_hat
f(θ) = 1+sin(π*θ)
2
1.5
1
0.5
0
-2
-1
0
1
2
f(θ)
θ
β = 0
β = 40
J_β(θ) = | y_d - f(θ) |^2 + β |θ|^2
120
100
80
60
40
20
0
-2
-1
0
1
2
J_β(θ)
θ

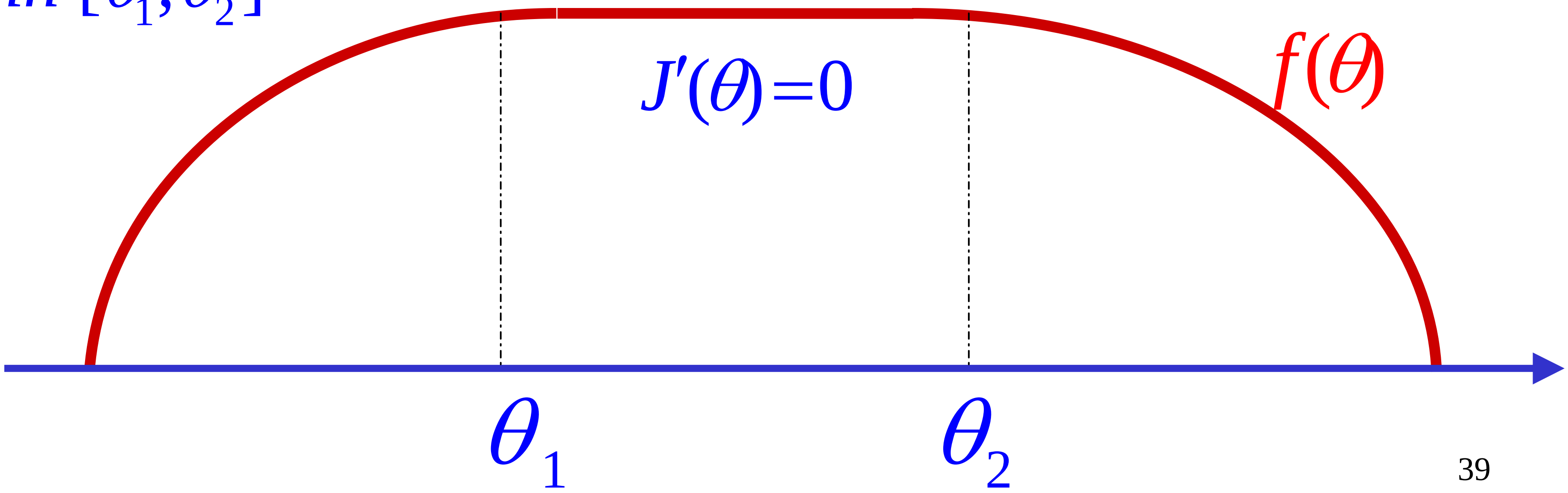
SENSITIVITY

How does $f(t,\theta) = \mathrm{C}\ z(t,\theta)$ *change with respect to* θ *and how does this affect the effort to minimize*

$$J(\theta) = \left| y_1 - f(\theta) \right|^2 \ ??$$

Recall that $J'(\theta) = 2(y_1 - f(\theta))(-f'(\theta))$ *and Newton*

$\theta^{k+1} = \theta^k - [J'(\theta^k)]^{-1} J(\theta^k)$ *stalls for initial values in* $[\theta_1, \theta_2]$



$So\ we\ are\ interested\ in\ \dfrac{\partial f}{\partial \theta} = C\ \dfrac{\partial z}{\partial \theta}$

which is obtained from general

sensitivity theory:

$$Example:\ For\ \frac{dz}{dt} = g(t, z, \theta),\ we\ find\ s(t) \equiv$$

$$\frac{\partial z(t, \theta^*)}{\partial \theta}\ satisfies\ \frac{ds(t)}{dt} = \left(\frac{\partial g}{\partial z}\right)^* s(t) + \left(\frac{\partial g}{\partial \theta}\right)^*$$

$$where\ \left(\frac{\partial g}{\partial z}\right)^* = \frac{\partial g}{\partial z}(t, z(t, \theta^*), \theta^*),$$

$$\left(\frac{\partial g}{\partial \theta}\right)^* = \frac{\partial g}{\partial \theta}(t, z(t, \theta^*), \theta^*)$$

APPROXIMATION/COMPUTATIONAL ISSUES

As we have noted, most observations have the form

$$f(t,\theta) = \mathcal{C}\, z(t,\theta),$$

where z is the solution of an ordinary or partial differential equation. In general, one cannot obtain these solutions in closed form even if θ is given. Thus one must turn to approximations and computational solutions.

For example, in the case of z satisfying an ODE

$$\frac{dz}{dt} = g(t, z, \theta),$$

one can apply finite difference techniques *to discretize the system, obtaining an algebraic system for* $z_k^N \approx z(t_k)$ *given by*

$$z_{k+1}^N = g^N(z_0^N, z_1^N, \ldots, z_k^N, \theta).$$

e.g., Runge–Kutta, predictor–corrector, stiff methods of Gear

Thus, one must use

$$f_k^N(\theta) = C\, z_k^N(\theta)$$

in

$$J^N(\theta) = \sum_{j=1}^{n} \left| \tilde{y}_j - f_j^N(\theta) \right|^2$$

which yields solutions $\hat{\theta}^N$.

Question: *What is relationship of* $\hat{\theta}^N$ *to* $\hat{\theta}$???

Convergence, preservation of stability, sensitivity, well posedness, etc., of problems, solutions ???

In the case of partial differential equation systems, one can introduce finite difference or finite element approximations.

Example: Finite elements ("linear elements") in dispersion equations – heat, population dispersal, molecular diffusion, etc.

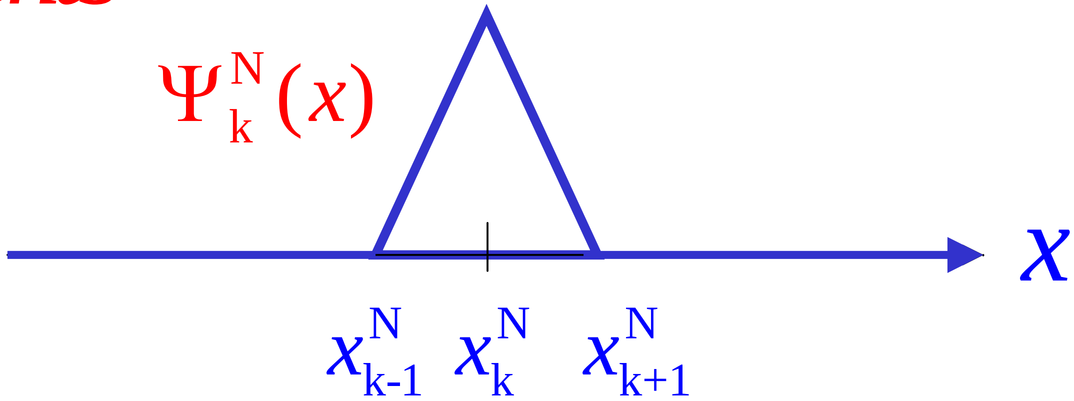
$$\frac{\partial u(t,x)}{\partial t} = \frac{\partial}{\partial x}\left(\theta(x)\frac{\partial u(t,x)}{\partial x}\right) + F(t,x)$$

Idea: *Look for approximate solutions of the form*

$$u^N(t,x)=\sum_{k=1}^{N} z_k^N(t)\Psi_k^N(x)$$

for a given set of basis elements $\left\{\Psi_k^N\right\}_{k=1}^{N}$, *leading to a system for* $z^N(t)=(z_1^N(t),z_2^N(t),\dots,z_N^N(t))$ *to be used in* $f^N(t,\theta)=\mathsf{C}^N z^N(t,\theta)$.

Linear Elements



leads to finite dimensional system

$$\frac{dz^N(t)}{dt} = A^N(\theta) z^N(t) + F^N(t)$$

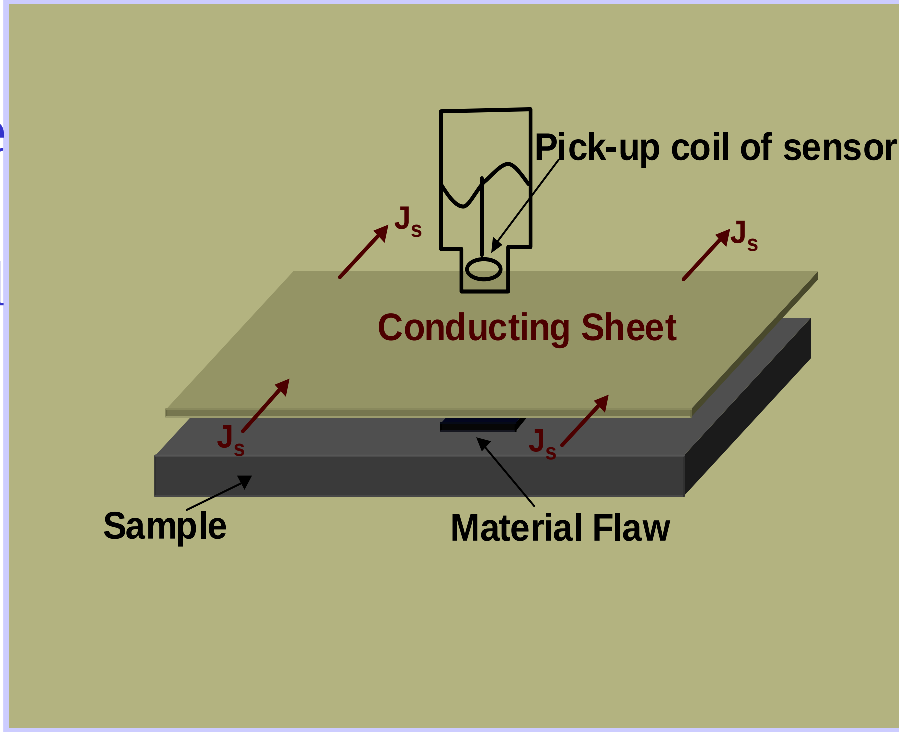
where

$$A^N(\theta) = \left(\int \theta(x) \Psi_i^N(x)' \Psi_j^N(x)' dx \right)$$

Finite elements generally result in large (dimension ~ 10,000-20,000) approximating systems!! These can be extremely time consuming in inverse problem calculations. So there is great interest in *model reduction techniques* that will result in substantial reduction in time! To illustrate one such technique (*Proper Orthogonal Decomposition*), we return to the eddy current based NDE example.

Computational Methodology for Eddy Current Based NDE Techniques

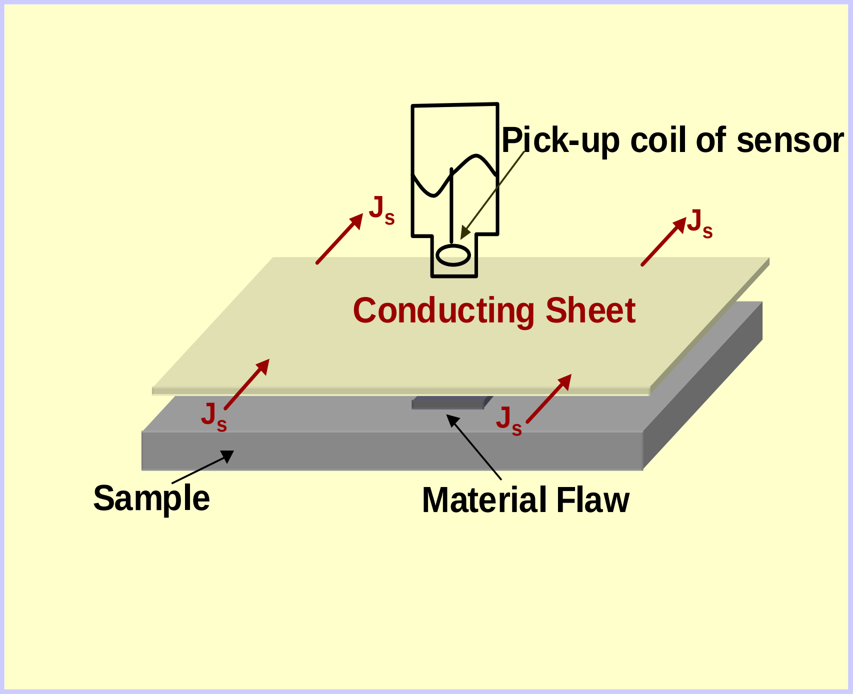
Develop fast on-line computational methods for use with highly sensitive magnetic flux sensors in detection of subsurface damages in portable, real time scanning devices for damage detection in conductive materials (fast scanners for NDE in aging aircraft, spacecraft and other structures).



Reduced order models (10 POD elements) to permit inverse problem calculations in 8 seconds resulting in 3 orders magnitude speed-up (computationally and experimentally validated)

Eddy Current Methods

- A conducting sheet carrying a uniform source current is placed near the sample to be examined.
- The current in the conducting sheet induces a current in the sample, called an eddy current.
- If a defect is present, it disrupts the flow of the eddy current.
- The disturbance in the eddy current manifests itself in the magnetic field data taken by the measuring device.



Maxwell's Equations in Phasor Form

Maxwell's Equations

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{D} = \rho$$

$$\nabla \times \mathbf{E} = -i\omega \mathbf{B}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + i\omega \mathbf{D}$$

Constitutive Laws

$$\mathbf{D} = \varepsilon \mathbf{E}$$

$$\mathbf{H} = \frac{1}{\mu} \mathbf{B}$$

Ohm's Law

$$\mathbf{J} = \sigma \mathbf{E}$$

where

- **B is the magnetic flux density in T**
- **D is the electric displacement in C/m^2**
- **E is the electric field intensity in V/m**
- **H is the magnetic field intensity in A/m**
- **J is the current density in A/m^2**
- **ρ is the electric charge density in C/m^3**
- **ω is the angular frequency in rad/s**
- **ε is the permittivity in F/m**
- **μ is the magnetic permeability in H/m**
- **σ is the electric conductivity in S/m**

Boundary Value Problem

The entire boundary value problem is given by

$$\nabla \times \left(\frac{1}{\mu(x,y)} \nabla \times \mathbf{A}(x,y) \right) = \left(\sigma(x,y) + i\omega\varepsilon(x,y) \right)\left(-i\omega\mathbf{A}(x,y) - \nabla\phi \right) \quad (x,y) \in \Omega,$$

$$I_{cs} = \int_{cs} \left(\sigma(x,y) + i\omega\varepsilon(x,y) \right)\left(-i\omega\mathbf{A}(x,y) - \nabla\phi \right) \cdot \mathbf{n}\, da \quad (x,y) \in cs$$

$$\nabla\phi = 0 \quad (x,y) \in \Omega \setminus cs$$

$$\mathbf{A}(x,-35mm) = \mathbf{0} = \mathbf{A}(x,35mm)$$

$$\nabla\mathbf{A}\cdot\mathbf{n}\big|_{(0mm,y)} = \mathbf{0} = \nabla\mathbf{A}\cdot\mathbf{n}\big|_{(50mm,y)}$$

for the magnetic vector potential $\mathbf{A}$ and scalar potential ϕ defined by

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -i\omega\mathbf{A} - \nabla\phi$$

Potential Difficulties in Inverse Problem

- **The ultimate goal is to determine the feasibility of using a portable sensing device in conjunction with inverse problem techniques to characterize a damage.**
- **The inverse problem is a computationally intensive iterative procedure in which the boundary value problem (BVP) must be solved possibly numerous times.**
- **Using standard finite element methods, the inverse problem would be extremely time consuming and therefore not practical in experimental settings.**
- **To decrease the computational time, one can use the reduced order POD (Proper Orthogonal Decomposition) methodology.**

POD Method

- ***Let q_j represent a damage and $A(q_j)$ denote the solution to the boundary value problem given damage q_j. Then the set of N_s snapshots is given by***

$$\left\{ A(\mathbf{q}_j) \right\}_{j=1}^{N_s}$$

- ***We seek POD basis elements Φ_i of the form***

$$\Phi_i = \sum_{j=1}^{N_s} V_i(j) A(\mathbf{q}_j)$$

such that each basis element Φ_i, $i=1,\ldots,N_s$ resembles the snapshots in the sense that it maximizes

$$\frac{1}{N_s} \sum_{j=1}^{N_s} \left| \left\langle A(\mathbf{q}_j), \Phi_i \right\rangle_{L^2(\Omega,\mathrm{C})} \right|^2$$

subject to $(\Phi_i, \Phi_i) = \| \Phi_i \|^2 = 1$.

Forming the POD Basis Elements

- *The coefficients $V_i(j)$ are found by solving the eigenvalue problem CV = λV where the covariance matrix C is given by*

$$[C]_{ij} = \frac{1}{N_s}\left\langle A(\mathbf{q}_i), A(\mathbf{q}_j)\right\rangle_{L^2(\Omega,\mathrm{C})}.$$

- *C is a Hermitian positive semi-definite matrix and hence possesses a complete set of orthogonal eigenvectors with corresponding non-negative real eigenvalues which can be ordered according to*

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{N_s} \geq 0.$$

- *The set of POD basis elements is given by* $\left\{\Phi_i\right\}_{i=1}^{N_s}$

  where

$$span\left\{\Phi_i\right\}_{i=1}^{N_s} = span\left\{A(\mathbf{q}_j)\right\}_{j=1}^{N_s}.$$

- *The reduced basis is given by*

$$\left\{\Phi_i\right\}_{i=1}^{N}$$

  where N is chosen so that

$$span\left\{\Phi_i\right\}_{i=1}^{N} \approx span\left\{A(\mathbf{q}_j)\right\}_{j=1}^{N_s}.$$

  which can be found by examining

$$\%\ energy = \sum_{j=1}^{N}\lambda_j \Big/ \sum_{j=1}^{N_s}\lambda_j$$

Approximation of A(q) Not in the Set of Snapshots

To approximate $A^N(q)$ where q is a given parameter not in the set $\{q_j\}_{j=1}^{N_s}$, we can use the approximation formula given by

$$A^N(\mathbf{q}) \equiv \sum_{k=1}^{N} \alpha_k(\mathbf{q})\Phi_k$$

where $\alpha_k(q)$ can be determined by one of the following:

1) ***POD/Galerkin Methods***

2) ***POD/Interpolation Method***

The POD/Galerkin method uses the equation which describes the system.

The POD/Interpolation methods only uses the value of $\alpha_k(q)$ for those damages parameters q in the set $\{q_j\}_{j=1}^{N_s}$. The equation describing the system is not involved.

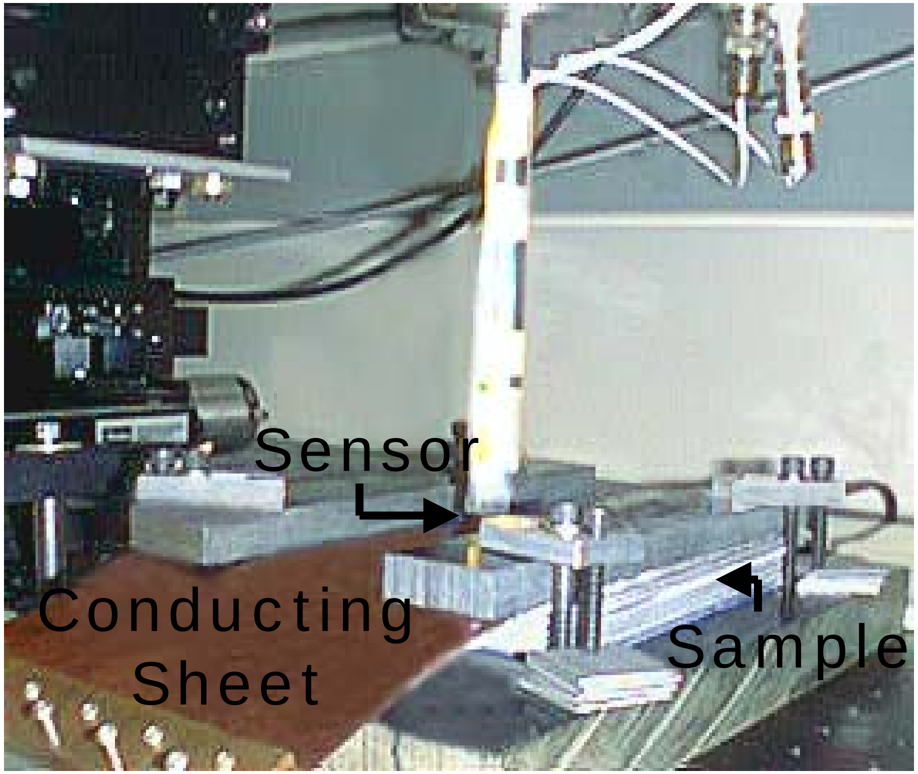
Computational Examples

- **Computational simulations were performed in which we estimated length, thickness, and depth separately and length and depth simultaneously.**
- **We generated "snapshots" of the magnetic vector potential, A, by using Ansoft Maxwell 2D Field Simulator(finite elements) to generate "data" across various damages.**
- **Simulated "data" was formed in the same way with random noise added to model random measurement error.**
- **In the parameter estimation problem, a scaled least squares criterion was used.**

Conclusions Based on Simulated Results

- **The methods were shown to be accurate and robust. Even with "data" containing considerable noise (10% in our example) the estimated parameters were a good representation of the actual parameters.**
- **Using a finite element package similar to Ansoft Maxwell 2D Field Simulator, over 7000 finite elements would have to be used in each forward run in the optimization problem where less than 10 POD basis elements are used while still obtaining extremely accurate results. This leads to a significant decrease in computational time.**
- **The methods were fast. The entire inverse problem took approximately 8 seconds. If one were using Ansoft Maxwell 2D Field Simulator, a single forward simulation would take on average 5-7 minutes. Thus we arrive at a speed up factor ranging from 750-1050, approximately a factor of 10^3.**

Experimental Setup



- **Sample:**

  17 layers of aluminum plates stacked on top of one another

- **Damage:**

  The damage is formed by cutting out a piece of one of the aluminum plates

- **Conducting Sheet:**

  Thin sheet of copper

- **Sensor:**

  GMR sensor

Results on Estimating Length with Experimental Data

Determination of Length at a Frequency of 500Hz

Depth (mm)	Length l^* (cm)	Est. Length (cm)	Relative Error
2	1.0	0.9397	6.03%
	1.5	1.6145	7.63
3	1.0	0.9428	5.72%
	1.5	1.4885	0.77%
4	1.0	0.9807	1.93%
	1.5	1.5334	2.23%

Determination of Length at a Frequency of 1kHz

Depth (mm)	Length l^* (cm)	Est. Length (cm)	Relative Error
2	1.0	1.0012	0.12%
	1.5	1.5109	0.73%
3	1.0	1.0090	0.90%
	1.5	1.6320	8.80%
4	1.0	1.0910	9.10%
	1.5	1.6613	10.76%

Results on Estimating Depth with Experimental Data

Determination of Depth with Fixed Length 1.0cm

Depth d^* (mm)	Frequency (Hz)	Est. Depth (mm)	Relative Error
2	250	0.9411	52.95%
	500	2.1919	9.59%
	1000	2.1191	5.96%
	2000	2.0479	2.39%
3	250	3.4827	16.09%
	500	2.8047	6.51%
	1000	2.9004	3.32%
	2000	2.9127	0.91%
4	250	3.4139	14.65%
	500	4.1277	3.19%
	1000	4.1865	4.66%
	2000	5.0469	26.17%

Results on Estimating Length and Depth with Experimental Data

Determination of Length and Depth at a Frequency of 500Hz

		Actual Length *l*		
		1.0cm	**1.5cm**	**2.0cm**
Actual Depth *d*	**2mm**	l = 1.0635 d = 2.3097	l = 1.8080 d = 1.8403	l = 1.5568 d = 1.9946
	3mm	l = 0.9065 d = 2.9522	l = 1.4612 d = 2.9759	l = 2.8565 d = 2.5408
	4mm	l = 1.2421 d = 4.2047	l = 1.5849 d = 3.9282	l = 1.6908 d = 3.9983

Relative Error for Determination of Length and Depth

		Actual Length *l*		
		1.0cm	**1.5cm**	**2.0cm**
Actual Depth *d*	**2mm**	R_l = 6.35% R_d = 15.48%	R_l = 20.53% R_d = 7.99%	R_l = 22.16% R_d = 0.27%
	3mm	R_l = 9.35% R_d = 1.59%	R_l = 2.59% R_d = 0.80%	R_l = 42.83% R_d = 15.31%
	4mm	R_l = 24.21% R_d = 5.12%	R_l = 5.66% R_d = 1.79%	R_l = 15.46% R_d = 0.12%

Overall Conclusions on POD

- **Taken as a whole, this work indicates that using the POD method in NDE research can be an attractive alternative to standard finite element methods, offering the potential for substantial savings in total computational time.**
- **Since the method is both fast and accurate, it suggests this method would be beneficial in real-time applications.**
- **It is possible to either snapshot on FEM simulations or experimental data when forming the POD basis elements and can obtain good results in both cases.**

SUMMARY REMARKS

1. **Two classes of problems (model/design driven-no data, and data driven)**
2. **In both classes, may need to introduce *variability/un-certainty* (recall PBPK, HIV examples) even when considering simple case of a single individual**
3. **If design/model driven efforts are successful (recall eddy current NDE example), most likely will lead to *validation experiments, data,* and necessitate develop-ment of *statistical models***
4. **There are significant issues, challenges, and methodology (well-posedness, regularization, approximation/computation, model reduction, etc.) that are important to consider in both classes of problems!**