Inverse Heat Conduction Problem Methods

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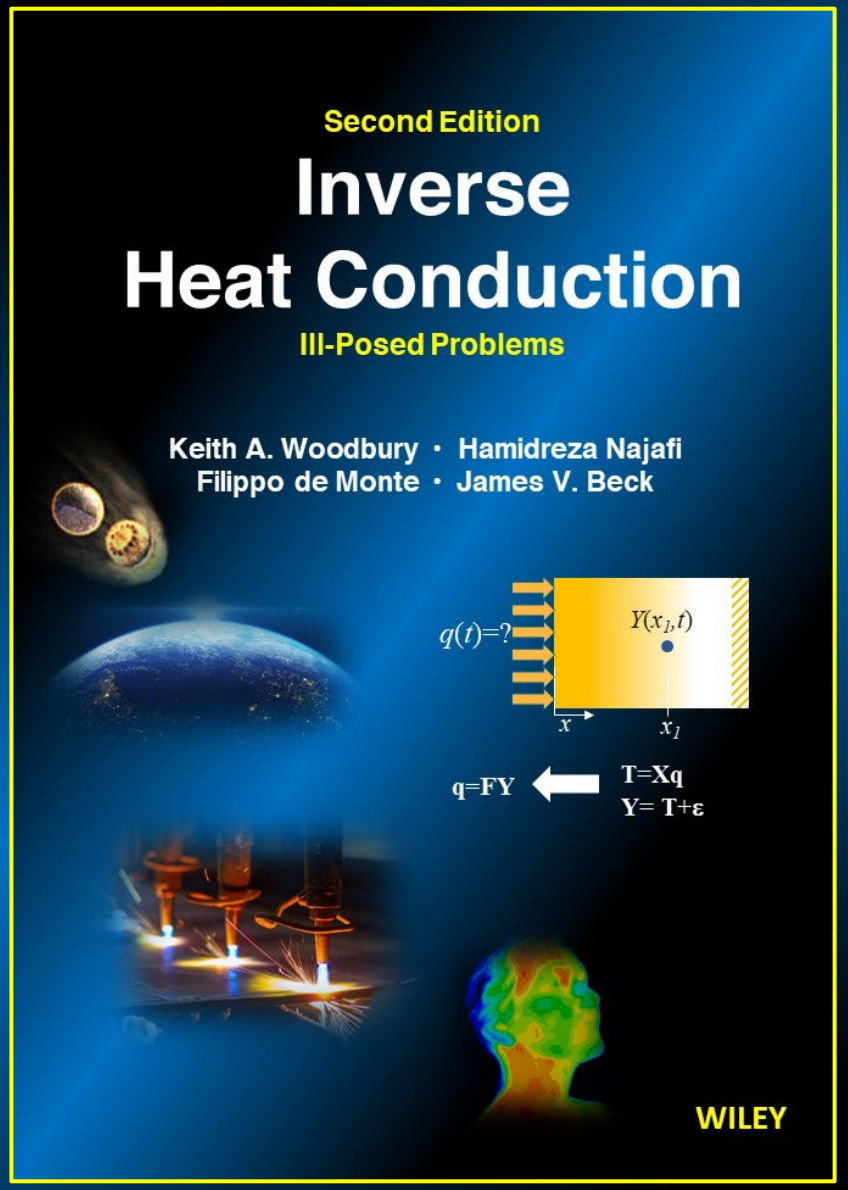
Second Edition
Inverse
Heat Conduction
Ill-Posed Problems
Keith A. Woodbury · Hamidreza Najafi
Filippo de Monte · James V. Beck
q(t)=?
Y(x1,t)
x
x1
q=FY
T=Xq
Y= T+ε
WILEY

Overview

1. Introduction
2. Direct Heat Conduction
   a) Superposition
   b) Discrete formulation
3. Ill-posedness and Regularization
4. IHCP Definition
5. Test Problem
6. IHCP Solution Techniques
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   b) Function Specification Method
   c) Tikhonov Regularization
   d) Gradient Methods – Conjugate Gradient
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7. Optimal Regularization
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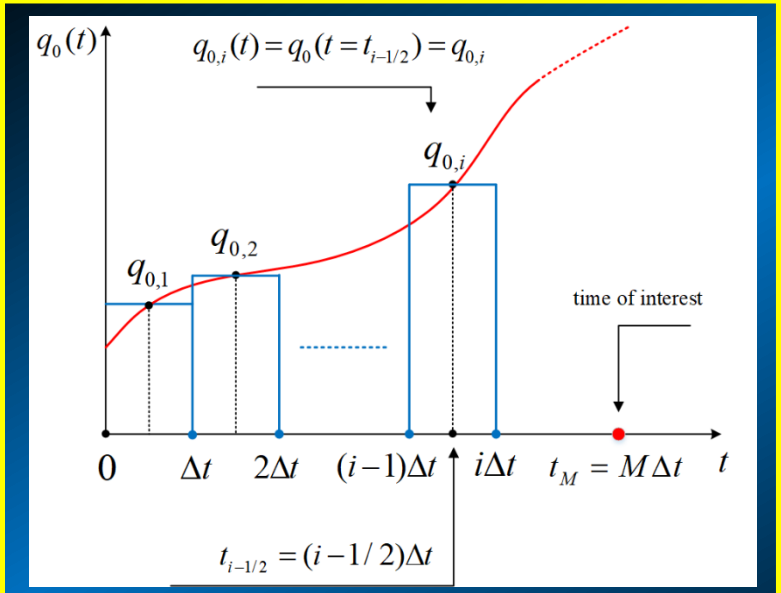
8. Summary

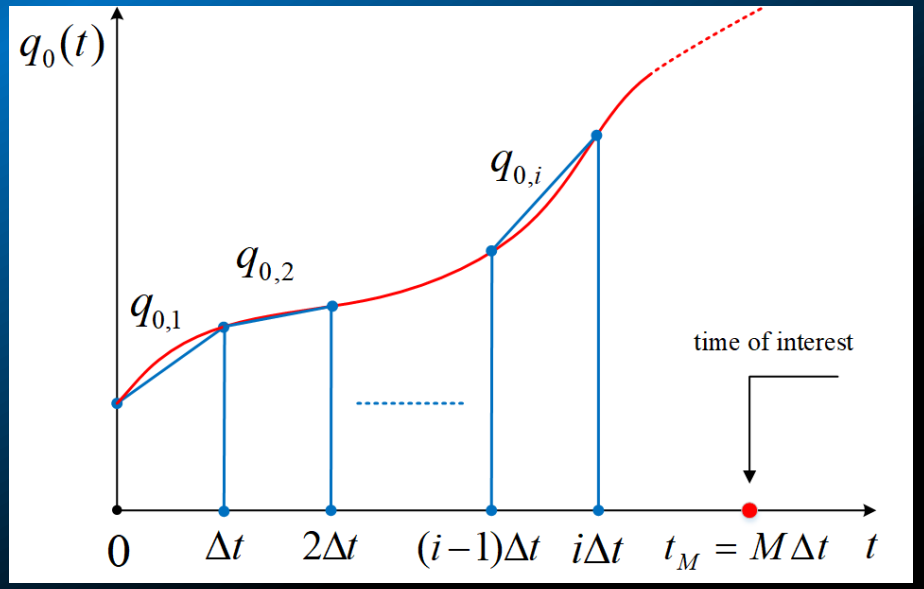
Introduction

Function Estimation vs. Parameter Estimation

- Parameter Estimation implies finding “a few” values
- Estimating a *function* implies determining a continuous variation of values
- The function might be approximated by a sequence of values



Piecewise constant



Piecewise linear

Direct and Inverse Problems

- (Alifanov, and others)
  - ➢Direct problems
    - ✓require determination of effects from known causes
  - ➢Inverse problems
    - ✓require determination of unknown causes based on observation of their effects

- In order to solve the inverse problem, a solution to the corresponding direct problem is needed

Direct (Forward) Heat Conduction Problem

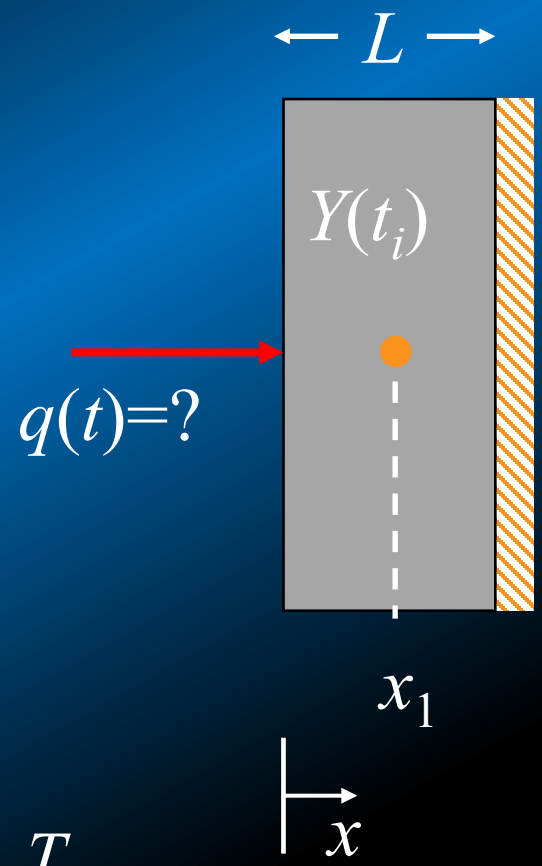
Linearity and Superposition

Mathematical Description

- Given: $\dfrac{\partial^2 T}{\partial x^2} = \dfrac{\partial T}{\partial t}, \qquad 0 \le x \le 1,\ t > 0$

$$-\left.\frac{\partial T}{\partial x}\right|_{x=0} = q(t) \qquad \frac{\partial T}{\partial x}(1,t) = 0$$

$$T(x,0) = 0$$



- Find $T(x,t)$ or maybe $T(x_1,t_i) = Y_i$.

- Note $x = \dfrac{x_d}{L}; \qquad t = \dfrac{\alpha t_d}{L^2}; \qquad q = \dfrac{q_d}{q_{ref}}; \qquad T = \dfrac{T_d}{q_{ref} L / k}$

Solution

- When the forcing function is constant $q(t) = \dfrac{q_c}{q_{ref}}$

$$\varphi(x,t) = T(x,t) = \frac{T_d(x,t)}{q_c L/k} = t + \frac{1}{3} - x + \frac{x^2}{2} - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}e^{-n^2\pi^2 t}\cos(n\pi x)$$

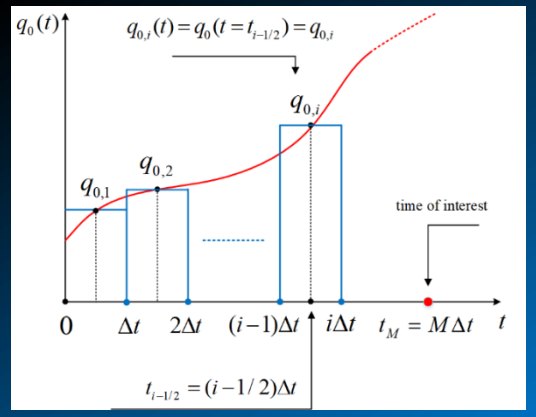
- When q(t) is a known function of time, superposition can be used to generate the solution from the kernel above.
  - A convolution integral results from Duhamel's theorem (or application of Green's functions)

$$T(x,t) = T_0 + \int_0^t q(\lambda)\frac{\partial\varphi(x,t-\lambda)}{\partial t}d\lambda$$

- The kernel function $\varphi(x,t)$ is the response to a unit surface disturbance of the same type (in this case, q)

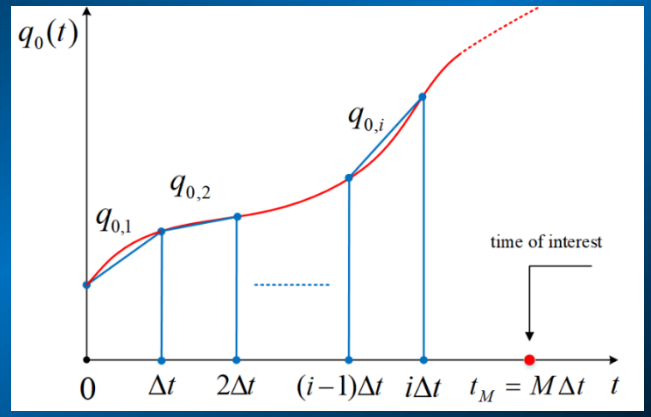
Discrete representation

- The function q(t) might be approximated by a sequence of values



Piecewise constant

or



Piecewise linear

- Then Duhamel's integral reverts to a summation

$$T(x_1, t_M) = T_0 + \sum_{n=1}^{M} q_n \Delta\varphi_{M-n}$$

$$\Delta\varphi_i = \varphi_{i+1} - \varphi_i$$

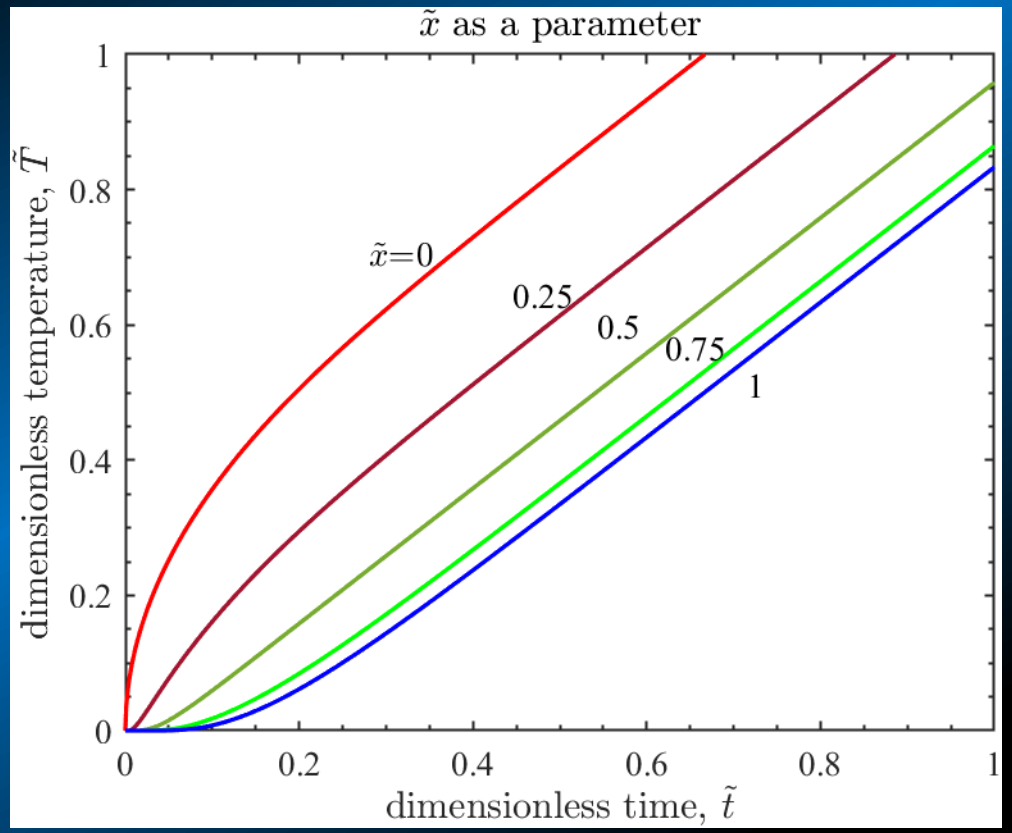
$$\varphi(x_1, t_i) = t_i + \frac{1}{3} - x_1 + \frac{1}{2}(x_1)^2 - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}e^{-n^2\pi^2 t}\cos(n\pi x_1)$$

piecewise constant *q*(*t*) is assumed for examples in this workshop

Kernel Function – Exact Solution

- For constant heat flux at x=0 (X22B10T0 problem)

$$\varphi(x,t) = T(x,t) = \frac{T_d(x,t)}{q_0 L/k} = t + \frac{1}{3} - x + \frac{x^2}{2} - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}e^{-n^2\pi^2 t}\cos(n\pi x)$$



Discrete Representation

- By writing a Duhamel's summation for discrete intervals of time, a matrix representation results

$$\{\mathbf{T}\} = [\mathbf{X}]\{\mathbf{q}\} + T_0\{\mathbf{1}\}$$

$$X_{ij} = \frac{\partial T_i}{\partial q_j}$$

where $\mathbf{X}$ is the *sensitivity matrix*

$$\mathbf{X} = \begin{bmatrix} \Delta\varphi_0 & 0 & \cdots & 0 \\ \Delta\varphi_1 & \Delta\varphi_0 & \ddots & 0 \\ \vdots & \vdots & \ddots & 0 \\ \Delta\varphi_M & \Delta\varphi_{M-1} & \cdots & \Delta\varphi_0 \end{bmatrix}$$

Lower-triangular Toeplitz matrix

$\Delta\varphi_i$ Depends on both the location x_1 and the time step $\Delta t = t_{i+1} - t_i$

Smaller values of $\Delta\varphi$ cause $|\mathbf{X}| \to 0$ and $\text{cond}(\mathbf{X}) \to \infty$

Importantly $\mathbf{T} = \mathbf{X}\mathbf{q}$ for homogeneous initial condition

Important points

- The magnitude of the entries of the **X** matrix should be as large as possible for strong sensitivity to the heat flux components
- Larger **X** matrix entries result from
  - sensors closer to the surface (smaller *x* coordinate)
  - larger time intervals between heat flux components (larger Δt)
- Example: For sensor at $x_d/L = 0.5$

0.0037	0	0	0	0
0.0194	0.0037	0	0	0
0.0267	0.0194	0.0037	0	0
0.0290	0.0267	0.0194	0.0037	0
0.0297	0.0290	0.0267	0.0194	0.0037

$$\alpha \Delta t_d / L^2 = 0.03$$

0.0231	0	0	0	0
0.0557	0.0231	0	0	0
0.0596	0.0557	0.0231	0	0
0.0600	0.0596	0.0557	0.0231	0
0.0600	0.0600	0.0596	0.0557	0.0231

$$\alpha \Delta t_d / L^2 = 0.06$$

Ill-posedness and Regularization

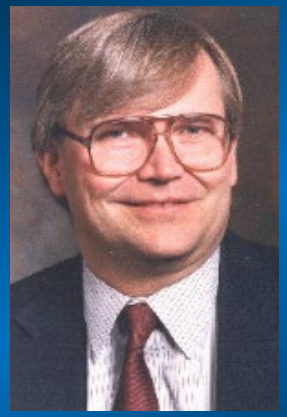
Ill-posedness

- (Hadamard) Mathematical problems are considered *ill-posed* if either
  - The solution is non-unique
  - The solution does not depend continuously on the data
- Most inverse problems fail on the second criteria

Ill-posedness

- Simple example (Hensel, 1991)

$$\begin{bmatrix} 1 & 1 \\ 1 & 1.01 \end{bmatrix} \begin{Bmatrix} a \\ b \end{Bmatrix} = \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$



  - Solution is a =1, b = 0
- Add 1% error to the "data" in the second equation

$$\begin{bmatrix} 1 & 1 \\ 1 & 1.01 \end{bmatrix} \begin{Bmatrix} a \\ b \end{Bmatrix} = \begin{Bmatrix} 1 \\ 1.01 \end{Bmatrix}$$

  - Now the solution is a = 0, b = 1!
- In the IHCP, errors are present in the temperature data due to measurement (both random errors (noise) and deterministic errors (bias))

Regularization

- To stabilize an ill-posed problem, some *regularization* is required
- Regularization is “any transformation of the original, ill-posed problem, to a ‘nearby’ stable problem” – Patti Lamm

Inverse Heat Conduction Problem

IHCP Definition

- Given:

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t}, \qquad 0 \le x \le 1, \; t > 0$$

$$\frac{\partial T}{\partial x}(1,t) = 0$$

$$T(x,0) = 0$$

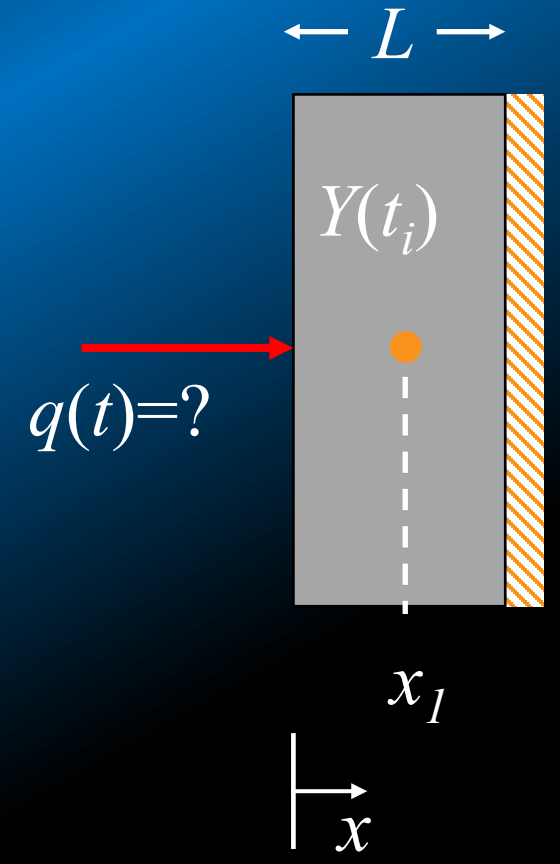
$$T(x_1,t_i) = Y_i \; .$$

- Find

$$q(t) = -\left.\frac{\partial T}{\partial x}\right|_{x=0}$$

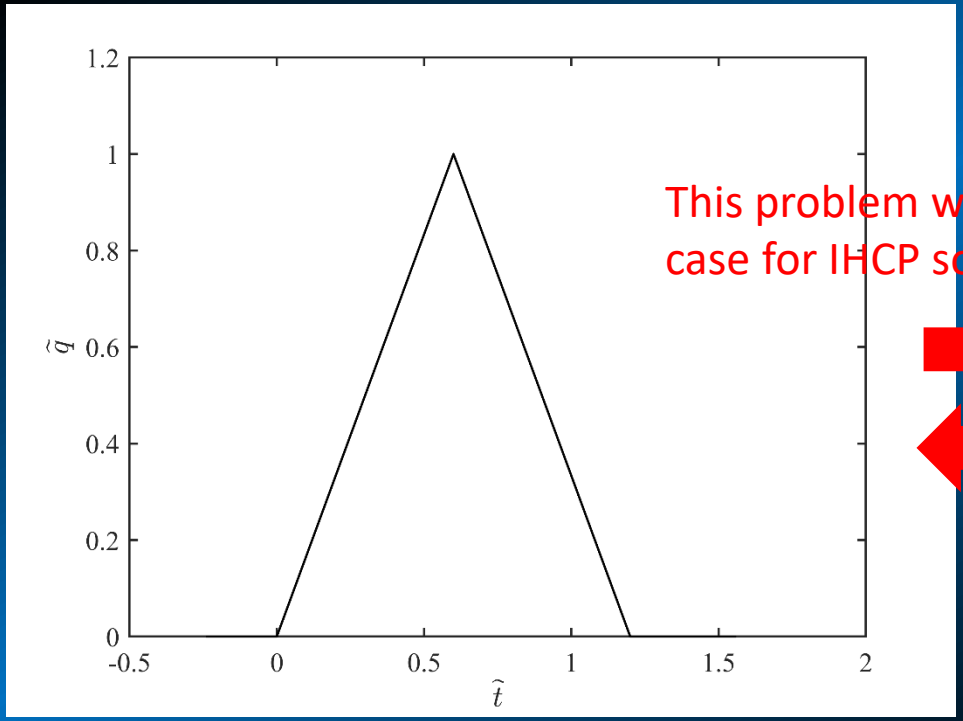
- Note

$$x = \frac{x_d}{L}; \qquad t = \frac{\alpha t_d}{L^2}$$

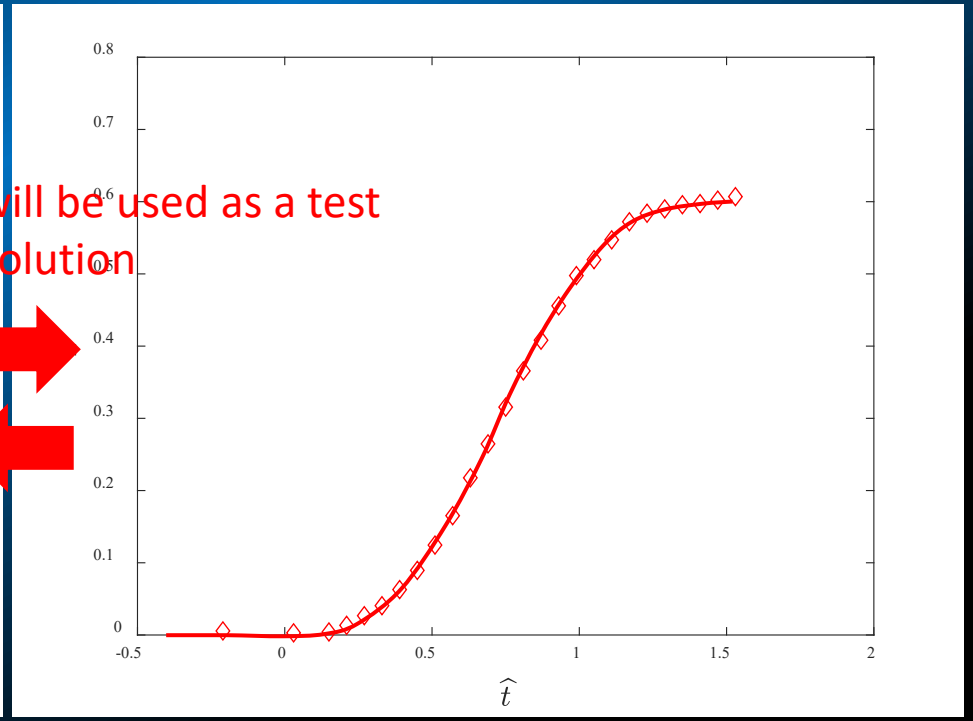


Test Problem

- Classic triangular-in-time heat flux applied at the surface
- An exact solution is used to generate “data”
- These “data” can be artificially poisoned with noise



This problem will be used as a test case for IHCP solution



IHCP – Solution Techniques

IHCP – Solution Techniques

- Exact Matching - Stolz Method
- Due to the ill-posedness of the IHCP, regularization is needed for stable solutions
  - Least-Squared-Error Matching Methods
    - Sequential Function Specification (Beck)
    - Tikhonov Regularization
    - Conjugant Gradient
  - Other methods
    - Truncated SVD
    - Neural Networks

Exact Matching

- Recall the forward problem solution for piecewise constant heat flux components

$$\mathbf{T} = \mathbf{X}\mathbf{q}$$

- If the model is exactly matched to measured data **Y** = **T**, then

$$\hat{\mathbf{q}} = \mathbf{X}^{-1}\mathbf{Y}$$

…and this works okay as long as $\mathbf{X}^{-1}$ is well-behaved

- Exact matching is what Stolz did, but not in a matrix form…

Stolz Method (1960)

- Based on exact matching of data at each
- Simple, but unstable for small time intervals
- Stoltz realized that the Lower-triangular nature of the matrix, **X**, meant that the components of the discrete **q** vector can be computed sequentially

$$\hat{q}_M = \frac{Y_M - \hat{T}_M\big|_{q_M=0}}{\varphi_1}$$

$$\hat{T}_M\big|_{q_M=0} = \sum_{i=1}^{M-1} \hat{q}_i \Delta\varphi_{M-i} + T_0$$

G. STOLZ, JR.
Senior Research Engineer, Heat and Mass Flow Analyzer Laboratory, Columbia University, New York, N. Y.

Numerical Solutions to an Inverse Problem of Heat Conduction for Simple Shapes

Stoltz Method (1960)

$$Y_1 = \Delta\varphi_0 q_1 \quad \Rightarrow \quad q_1 = \frac{Y_1}{\Delta\varphi_0}$$

$$Y_2 = \Delta\varphi_1 q_1 + \Delta\varphi_0 q_2 \quad \Rightarrow \quad q_2 = \frac{Y_2 - \Delta\varphi_1 q_1}{\Delta\varphi_0}$$

$$Y_3 = \Delta\varphi_2 q_1 + \Delta\varphi_1 q_2 + \Delta\varphi_0 q_3 \quad \Rightarrow \quad q_3 = \frac{Y_3 - \left(\Delta\varphi_2 q_1 + \Delta\varphi_1 q_2\right)}{\Delta\varphi_0}$$

$$\vdots$$

$$\Rightarrow \quad \text{etc...}$$

- Sequential (time marching)

$$\hat{q}_M = \frac{Y_M - \hat{T}_M\Big|_{q_M=0}}{\Delta\varphi_0} \qquad \hat{T}_M\Big|_{q_M=0} = \sum_{i=1}^{M-1} \hat{q}_i \Delta\varphi_{M-i} + T_0$$

Stolz Method - Example

- Consider the triangular heat flux with $\Delta t = 0.06$
- The first few simulated measurements are:

  $\mathbf{Y}$ ={0.005601, -0.000591, -0.000814, -0.002049, 0.002952}

  (these should be zero except for measurement noise added)
- The first few φ and $\Delta\varphi$ values are

  $\boldsymbol{\varphi}$ ={0.000786, 0.014887, 0.047584, 0.092297, 0.143824}

  $\Delta\boldsymbol{\varphi}$ **={**0.000786, 0.014102, 0.032697, 0.044713, 0.051527}

Stolz Method - Example

$$q_1 = \frac{Y_1}{\Delta\varphi_0} = \frac{0.00560}{0.000786} = 7.13$$

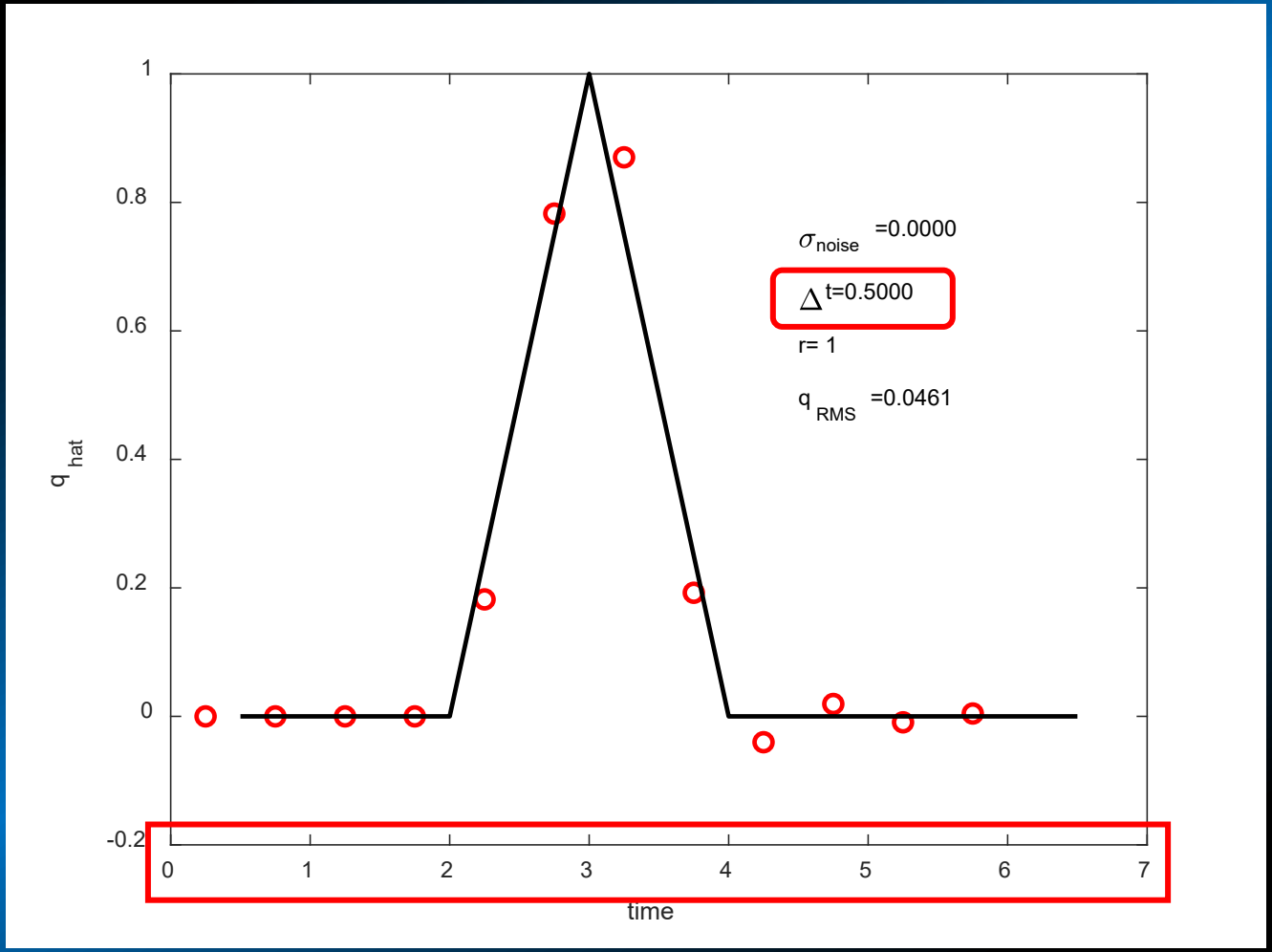
$$q_2 = \frac{Y_2 - \Delta\varphi_1 q_1}{\Delta\varphi_0} = \frac{-0.000591 - 0.01410 \times (7.13)}{0.000786} = -128.7$$

$$q_3 = \frac{Y_3 - \left(\Delta\varphi_2 q_1 + \Delta\varphi_1 q_2\right)}{\Delta\varphi_0} = \frac{-0.000814 - (0.032697 \times 7.13 + 0.01410 \times (-128.7)}{0.000786} = 2011$$

etc...

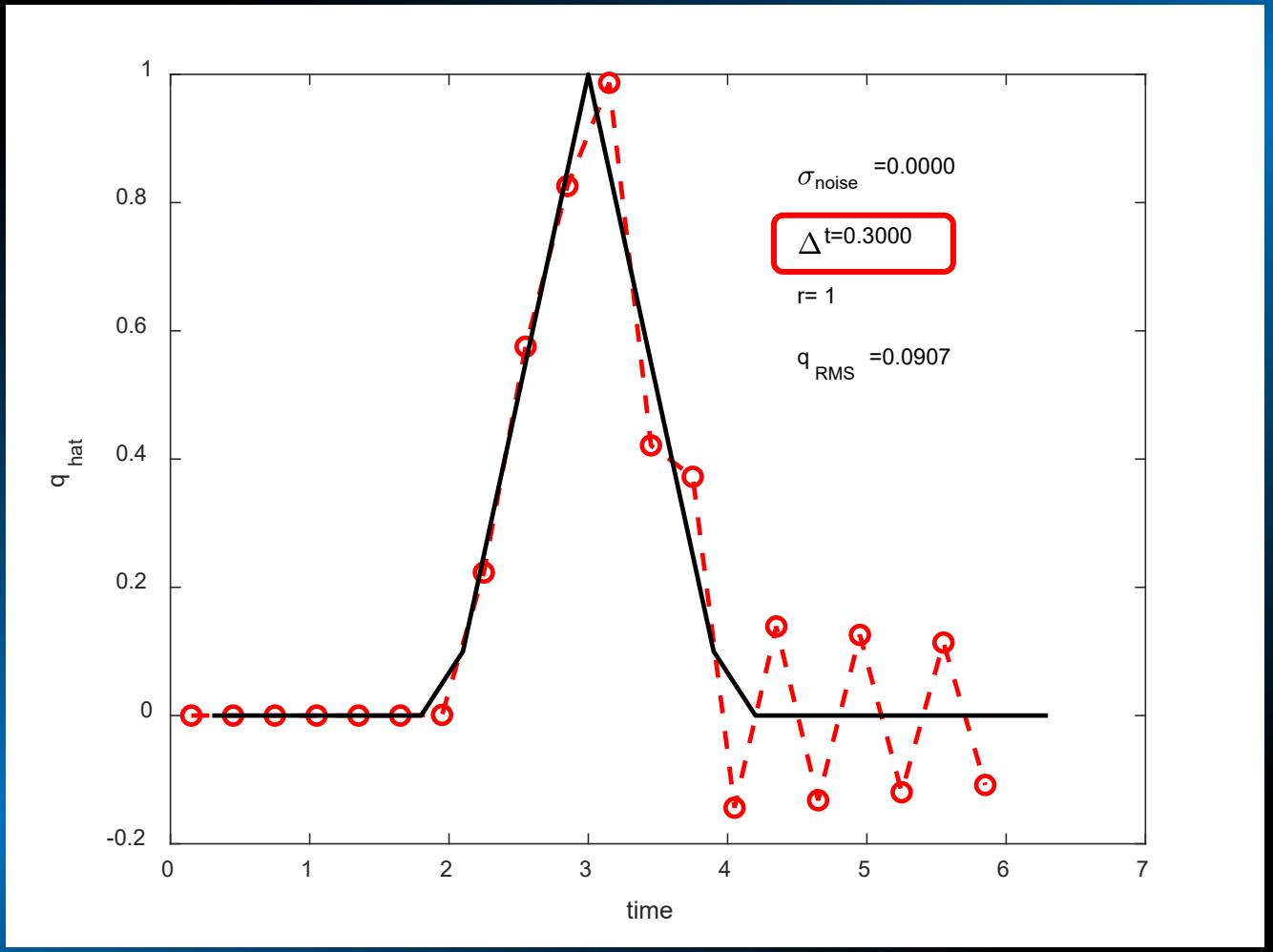
- Method is unstable for this small $\Delta t = 0.06$
- Larger time steps will stabilize calculations but with loss of resolution of $q(t)$

Stoltz Method – Example



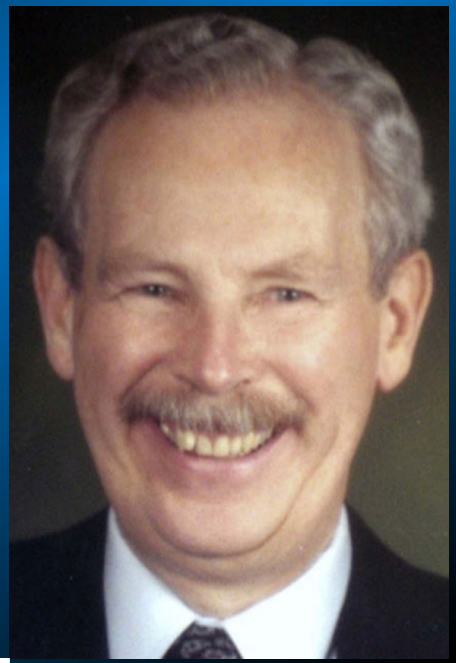
…to illustrate larger time steps time scale is changed for this Example

Stoltz Method – Example



Beck's Sequential Method

- Beck's innovation: add more data to the sequential procedure of Stoltz without adding additional unknowns



NUCLEAR ENGINEERING AND DESIGN 7 (1968) 170-178. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

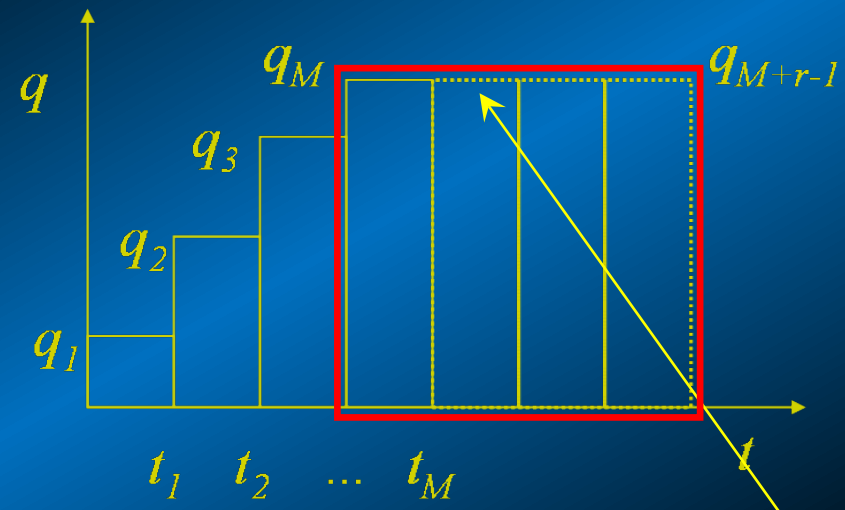
SURFACE HEAT FLUX DETERMINATION USING AN INTEGRAL METHOD

James V. BECK
Department of Mechanical Engineering and
Division of Engineering Research, Michigan State University,
East Lansing, Michigan 48823, *USA*

Received 5 December 1967

Beck's Sequential Method

- Assume a functional form for $q(t)$, typically piecewise constant
- Consider "r" future time steps of data
- Minimize



$$S = \sum_{i=1}^{r} \left(Y_{M+i-1} - T_{M+i-1} \right)^2 = \left(\mathbf{Y} - \mathbf{T} \right)^T \left(\mathbf{Y} - \mathbf{T} \right)$$

Adds more data

Without more unknowns

- *Temporarily* hold q_M constant over *"r"* time steps

Beck's Sequential Method

- By assuming *temporarily* that the heat flux variation is unchanged over the "*r* " times

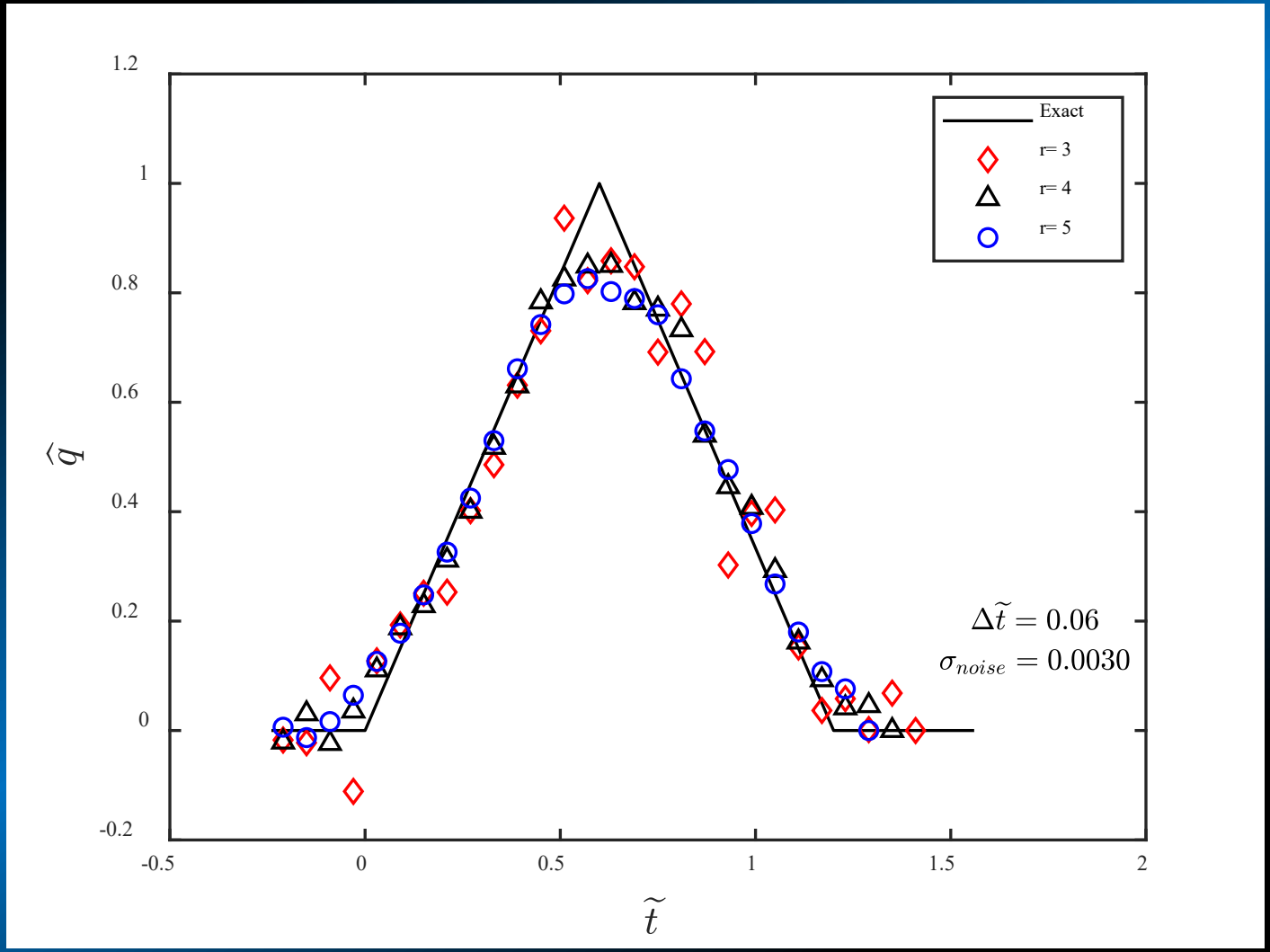
$$\hat{q}_M = \frac{\sum_{i=1}^{r} \varphi_i \left(Y_{M+i-1} - \hat{T}_{M+i-1} \right)}{\sum_{i=1}^{r} \varphi_i^2} = \sum_{i=1}^{r} K_i \left(Y_{M+i-1} - \hat{T}_{M+i-1} \right); \qquad K_i = \frac{\varphi_i}{\sum_{i=1}^{r} \varphi_i^2}$$

  as before

$$\hat{T}_{M+i-1} = \sum_{j=1}^{M-1} \hat{q}_j \Delta\varphi_{(M+i-1)-j}$$

- Compute each q_M in turn, then proceed to the next time step (M ← M+1)

Beck's Sequential Method - Example



Tikhonov Regularization

- Add a stabilizing (regularizing) penalty term to the sum of squares
  - Zeroth order: penalty proportional to the function value
  - First order: penalty proportional to the first (time) derivative
  - Second order: penalty proportional to the second (time) derivative
- One or more orders can be used.
- Typically, only zeroth or first order is used

SOLUTION OF INCORRECTLY FORMULATED PROBLEMS AND THE REGULARIZATION METHOD

A. N. TIHONOV

Tikhonov Regularization – Discrete Form

- Zeroth order

$$S = \left(\mathbf{Y} - \mathbf{X}\mathbf{q}\right)^T \left(\mathbf{Y} - \mathbf{X}\mathbf{q}\right) + \alpha_0 \mathbf{q}^T \mathbf{q}$$

- First order

$$S = \left(\mathbf{Y} - \mathbf{X}\mathbf{q}\right)^T \left(\mathbf{Y} - \mathbf{X}\mathbf{q}\right) + \alpha_1 \mathbf{q}^T \mathbf{H}_1^T \mathbf{H}_1 \mathbf{q}$$

- Second order

$$S = \left(\mathbf{Y} - \mathbf{X}\mathbf{q}\right)^T \left(\mathbf{Y} - \mathbf{X}\mathbf{q}\right) + \alpha_2 \mathbf{q}^T \mathbf{H}_2^T \mathbf{H}_2 \mathbf{q}$$

Tikhonov Regularization – Discrete Form

- First Order

$$\mathbf{H}_1 = \begin{bmatrix} -1 & 1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & 1 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 1 \\ 0 & 0 & \cdots & 0 & 0 & 0 \end{bmatrix}$$

➢Approximates first derivative

- Second Order

$$\mathbf{H}_2 = \begin{bmatrix} 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 \end{bmatrix}$$

➢Approximates second derivative

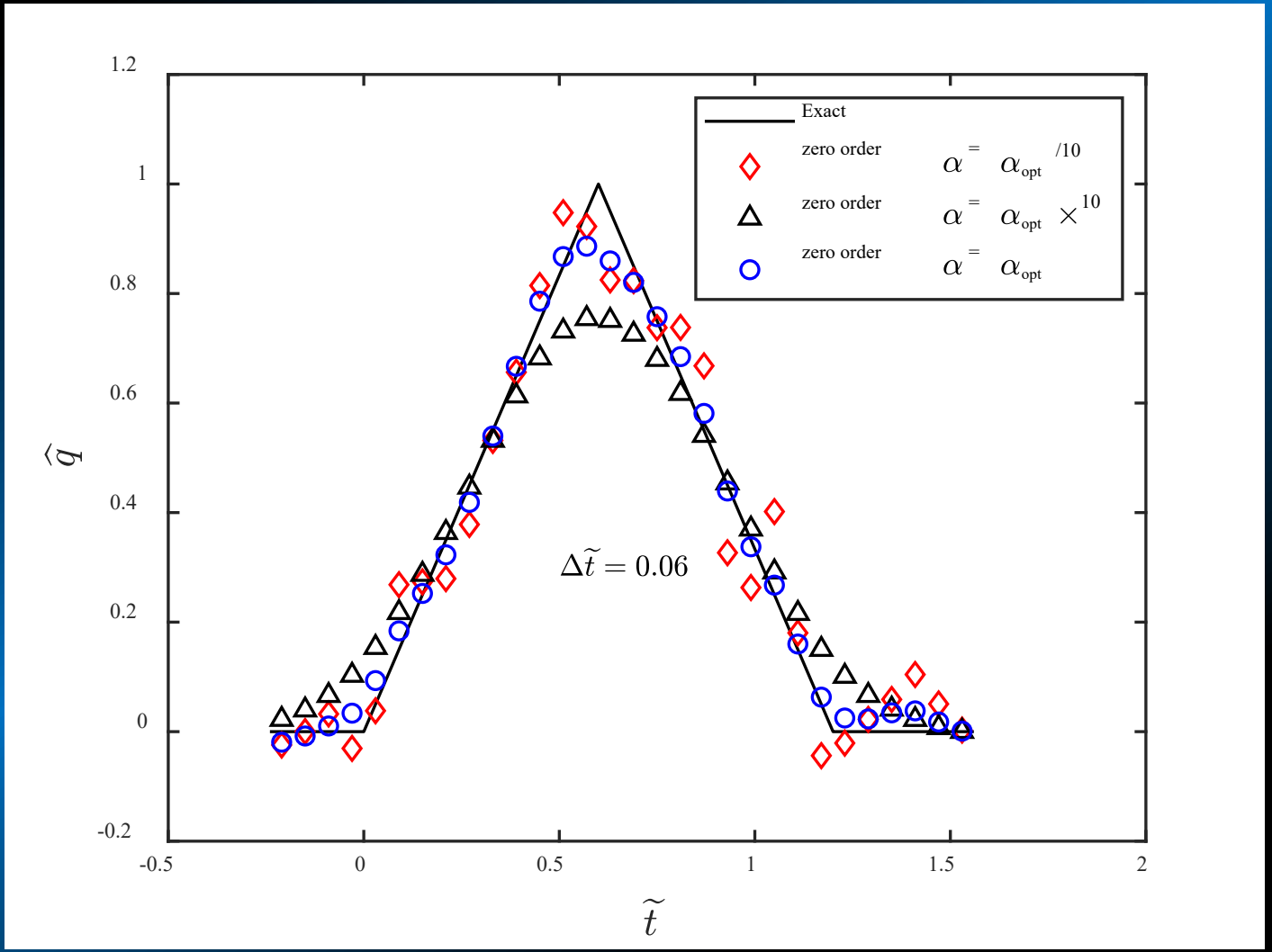
Tikhonov Regularization

- Minimizing the *S* function gives the estimator for the heat flux vector

$$\hat{\mathbf{q}} = \left(\mathbf{X}^T\mathbf{X} + \alpha_0\mathbf{I}\right)^{-1}\mathbf{X}^T\mathbf{Y} = \mathbf{F}\mathbf{Y}; \quad \mathbf{F} = \left(\mathbf{X}^T\mathbf{X} + \alpha_0\mathbf{I}\right)^{-1}\mathbf{X}^T$$

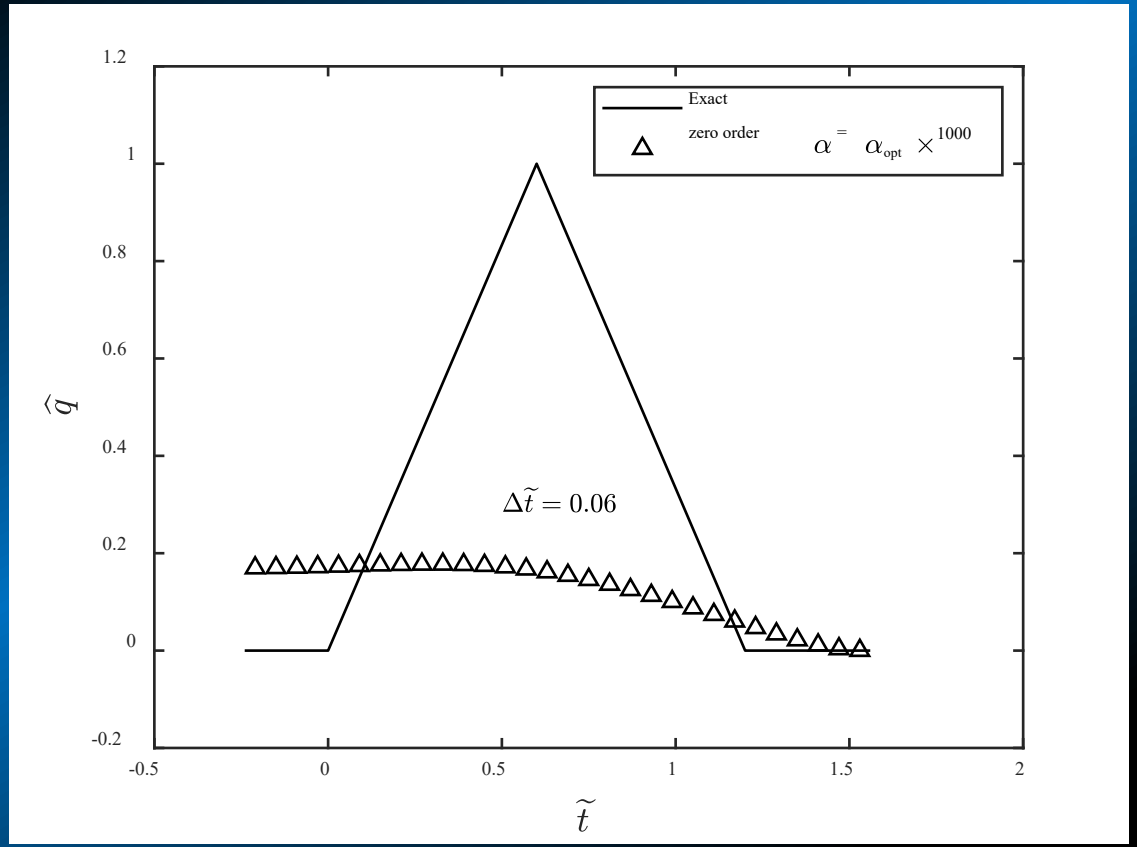
- The matrix **F** is identified as the *Filter Matrix*, which defines the mapping from measured temperatures (**Y**) to heat fluxes (**q**)
- Note that all heat flux components are computed simultaneously ("whole domain" method)

Tikhonov Regularization Example – Zeroth Order

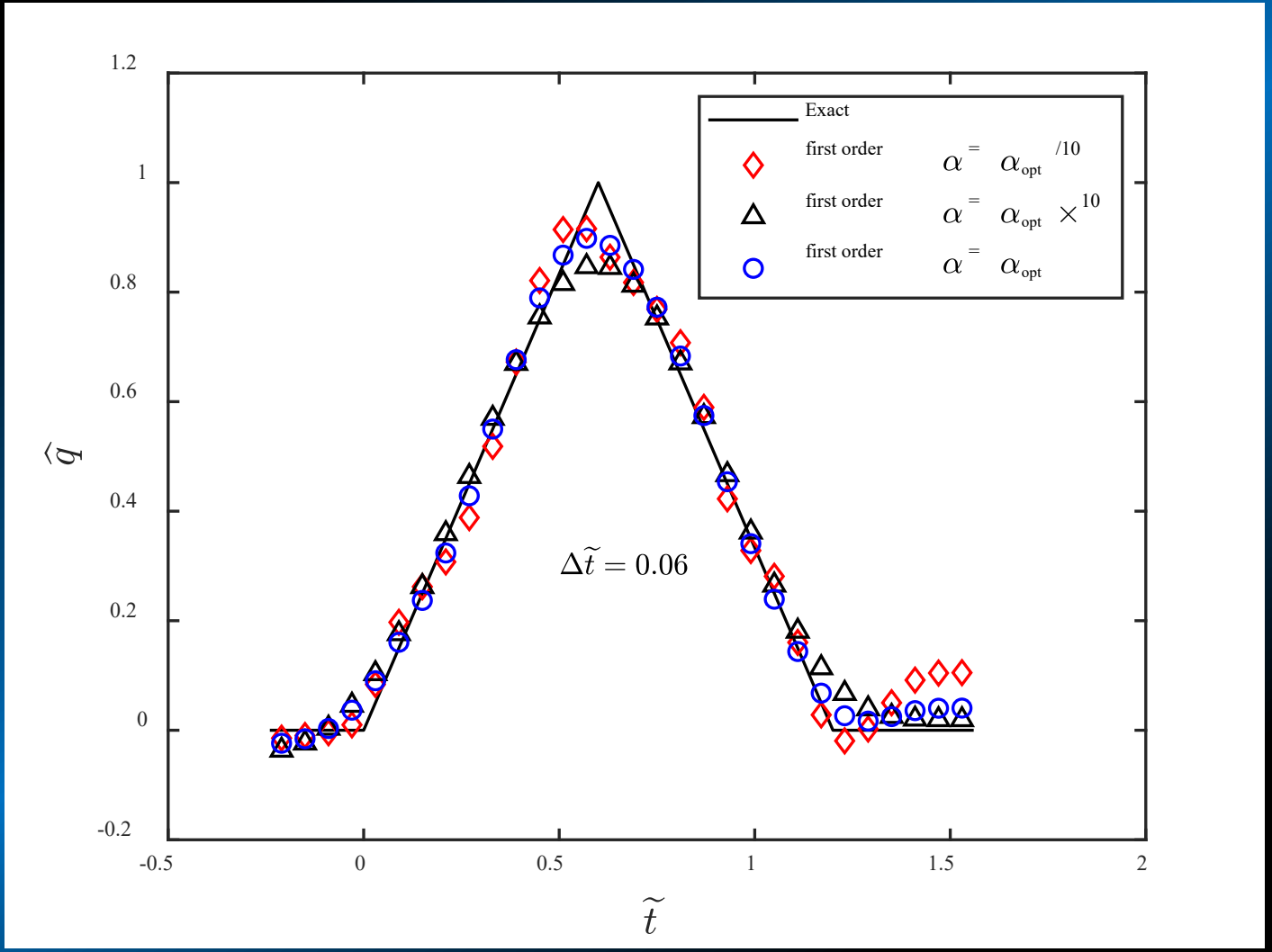


Tikhonov Regularization Example – Zeroth Order

- Effect of extreme over-regularization is bias of $q(t)$ toward zero

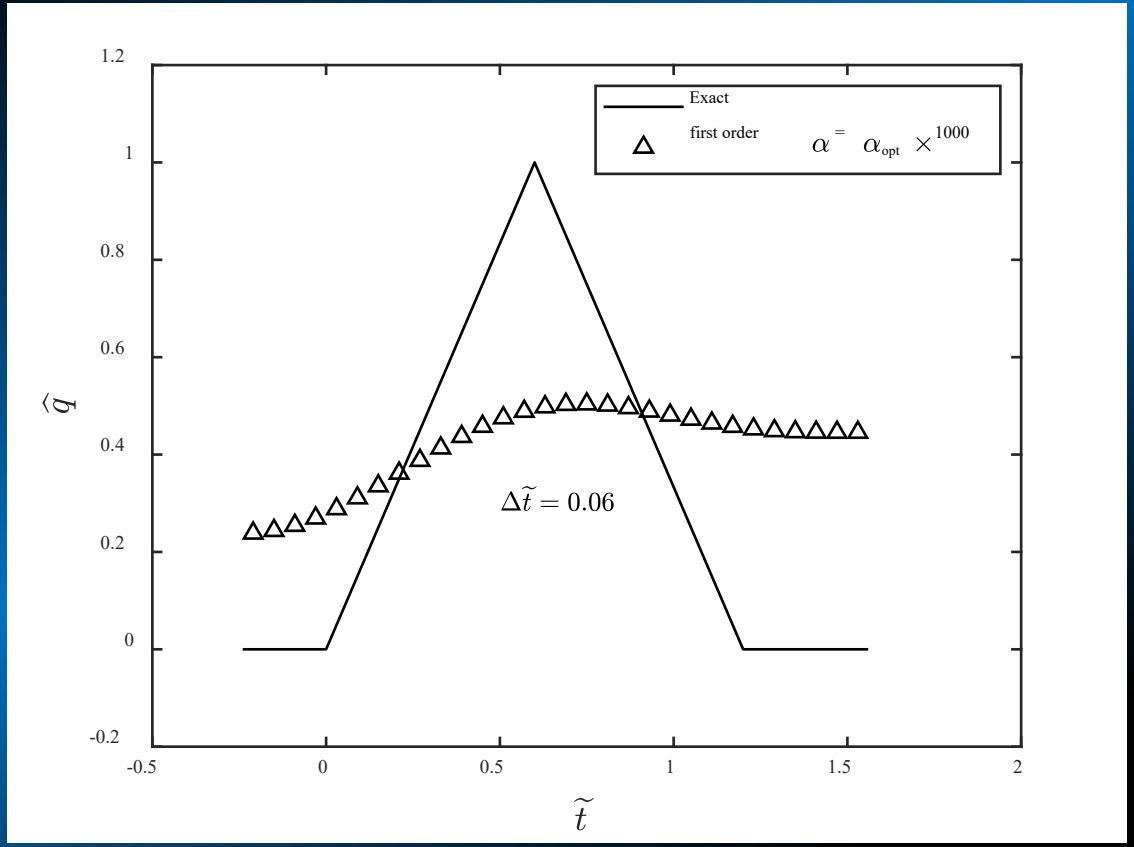


Tikhonov Regularization Example – First Order



Tikhonov Regularization Example – First Order

- Effect of extreme over-regularization is bias $q(t)$ toward a constant value



Conjugate Gradient Method

- Family of iterative methods to minimize *S*
  - Applicable to non-linear, as well as linear, cases
- Minimize

$$S(\mathbf{q}) = (\mathbf{Y} - \mathbf{X}\mathbf{q})^T (\mathbf{Y} - \mathbf{X}\mathbf{q})$$

- From the present estimate for $\mathbf{q}^{(k)}$, an improved estimate is formed as

$$\mathbf{q}^{(k+1)} = \mathbf{q}^{(k)} + \rho^{(k)}\mathbf{w}^{(k)}$$

- Various methods result for different choices of the *descent direction* $\mathbf{w}^{(k)}$ and *descent length* (step size) $\rho^{(k)}$

Conjugate Gradient Methods

- Steepest Descent

$$\mathbf{w}^{(k)} = -\nabla S^{(k)} = +2\mathbf{X}^T\left(\mathbf{Y} - \mathbf{X}\mathbf{q}^{(k)}\right)$$

$$\rho^{(k)} = Arg\min_{\rho>0} S\left(\mathbf{q}^{(k)} + \rho\mathbf{w}^{(k)}\right)$$

"go as far as you can in the direction of $\mathbf{w}^{(k)}$ to the minimum of S"

$$= -\frac{1}{2}\frac{\left(\mathbf{Y} - \mathbf{X}\mathbf{q}^{(k)}\right)^T \mathbf{X}\mathbf{X}^T\left(\mathbf{Y} - \mathbf{X}\mathbf{q}^{(k)}\right)}{\left(\mathbf{Y} - \mathbf{X}\mathbf{q}^{(k)}\right)^T \mathbf{X}\mathbf{X}^T\mathbf{X}\mathbf{X}^T\left(\mathbf{Y} - \mathbf{X}\mathbf{q}^{(k)}\right)}$$

Regularizing parameter is the final iteration number, *k*

Conjugate Gradient Methods

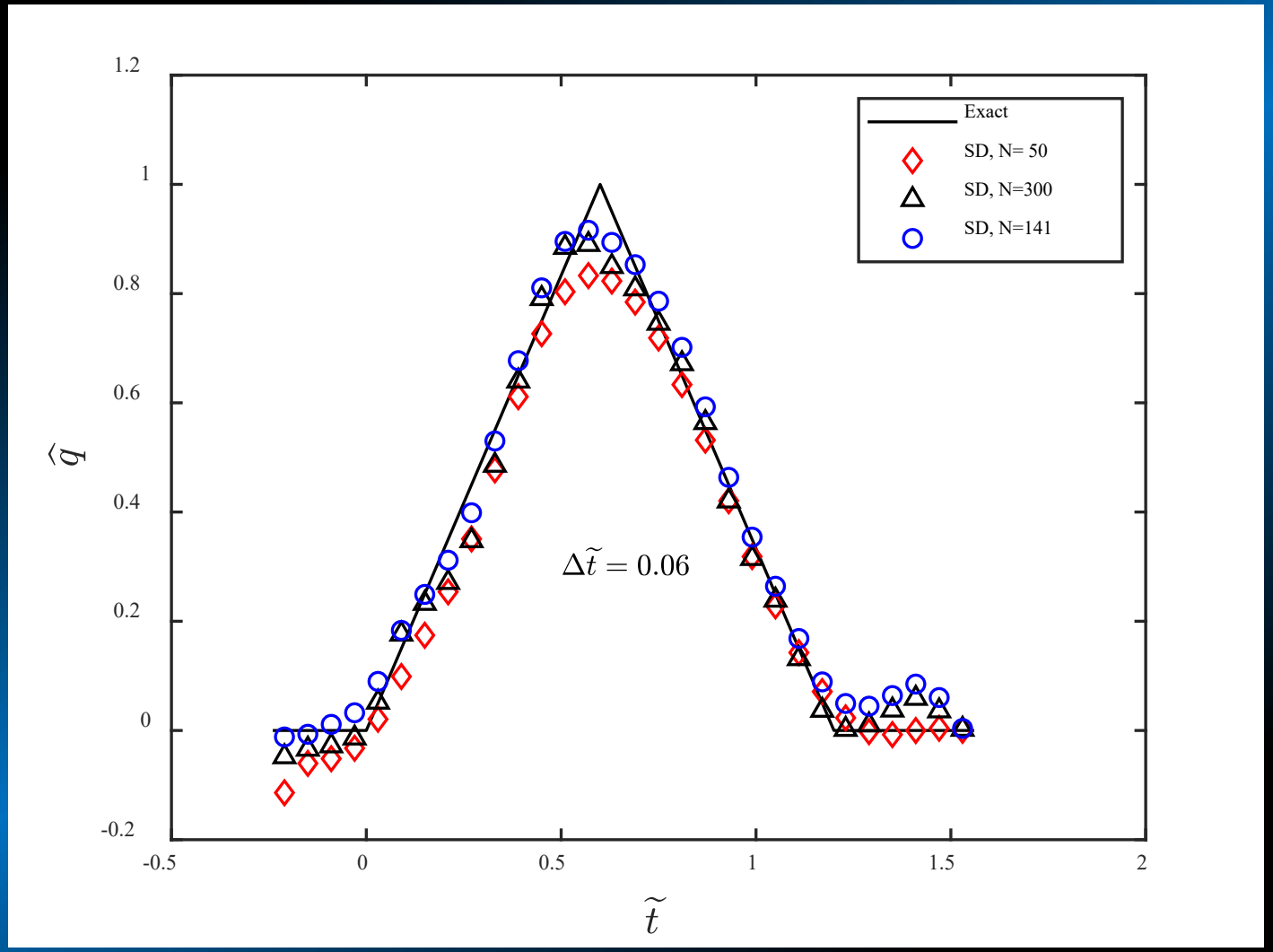
- Fletcher-Reeves algorithm

$$\mathbf{w}_k = \begin{cases} 2\mathbf{X}^T\left(\mathbf{Y}-\mathbf{X}\mathbf{q}_k\right) & k=1 \\ 2\mathbf{X}^T\left(\mathbf{Y}-\mathbf{X}\mathbf{q}_k\right)\dfrac{\left\|2\mathbf{X}^T\left(\mathbf{Y}-\mathbf{X}\mathbf{q}_k\right)\right\|^2}{\left\|2\mathbf{X}^T\left(\mathbf{Y}-\mathbf{X}\mathbf{q}_{k-1}\right)\right\|^2} & k>1 \end{cases}$$

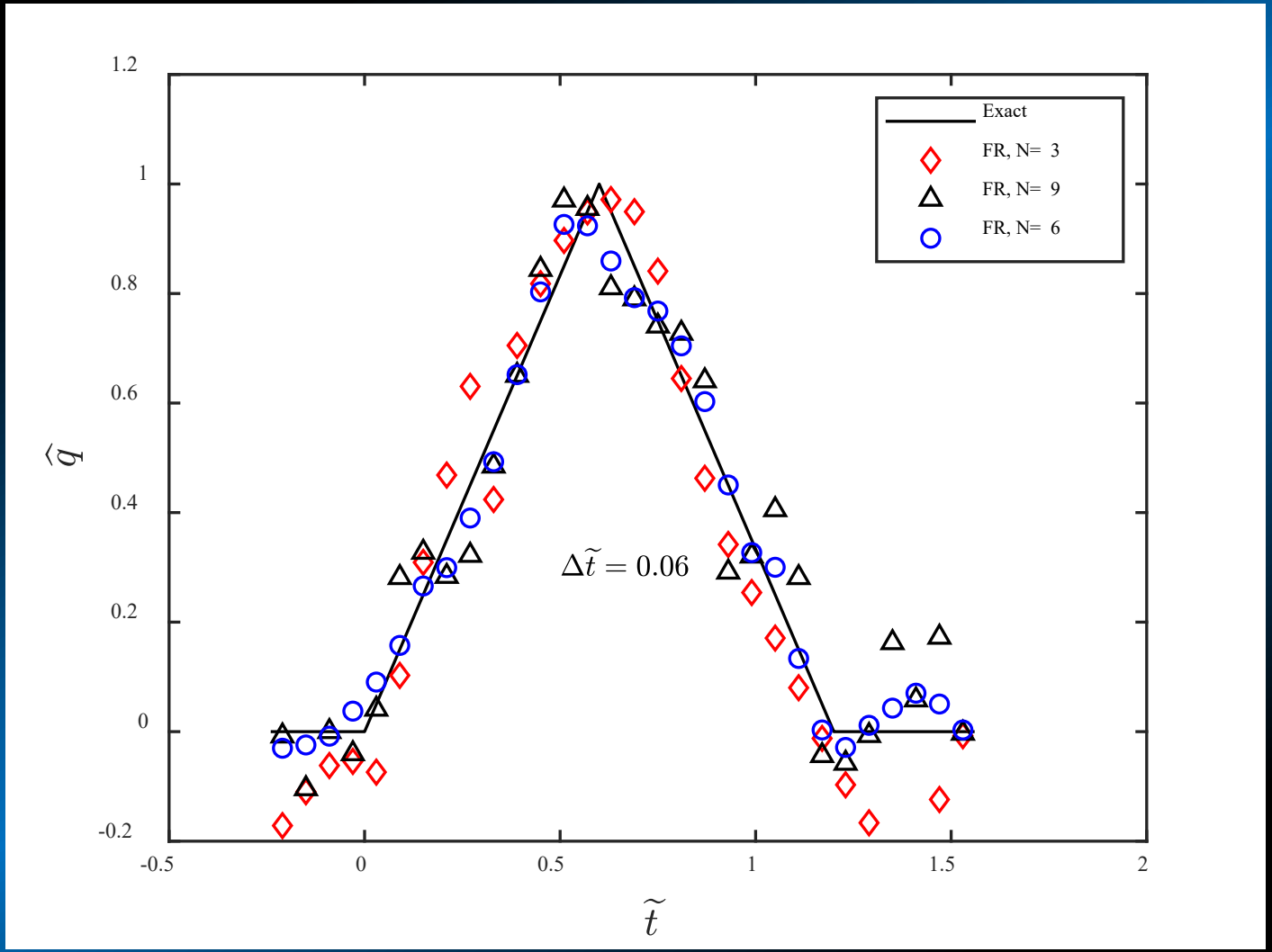
$$\rho_k = -\frac{\left(\mathbf{Y}-\mathbf{X}\mathbf{q}_k\right)^T\mathbf{X}\mathbf{w}_k}{\left\|\mathbf{X}\mathbf{w}_k\right\|^2}$$

- Other methods
  - Polak-Ribiere
  - Hestenes-Stiefel

Steepest Descent - Example



Fletcher-Reeves – Example



Singular Value Decomposition

- Solve directly (as in the Naïve approach)

$$\mathbf{q} = \mathbf{X}^{-1}\mathbf{Y}$$

  but, use *singular value decomposition* to invert the $\mathbf{X}$ matrix

- The SVD of a matrix is

$$SVD(\mathbf{X}) = \mathbf{U}\mathbf{W}\mathbf{V}^T = \mathbf{U}diag(w_j)\mathbf{V}^T$$

  where $diag(w_j)$ is a diagonal matrix of the *singular values* of $\mathbf{X}$, and $\mathbf{U}$ and $\mathbf{V}^T$ are orthogonal matricies

- Then

$$\mathbf{X}^{-1} = \mathbf{V}diag\left(1/w_j\right)\mathbf{U}^T$$

Truncated SVD (TSVD)

- The inverse of the matrix is approximated by eliminating the near-zero values of $\mathbf{W}$

$$\mathbf{q} = \mathbf{V} diag\left(1/w_j\right)\mathbf{U}^T\mathbf{Y}$$

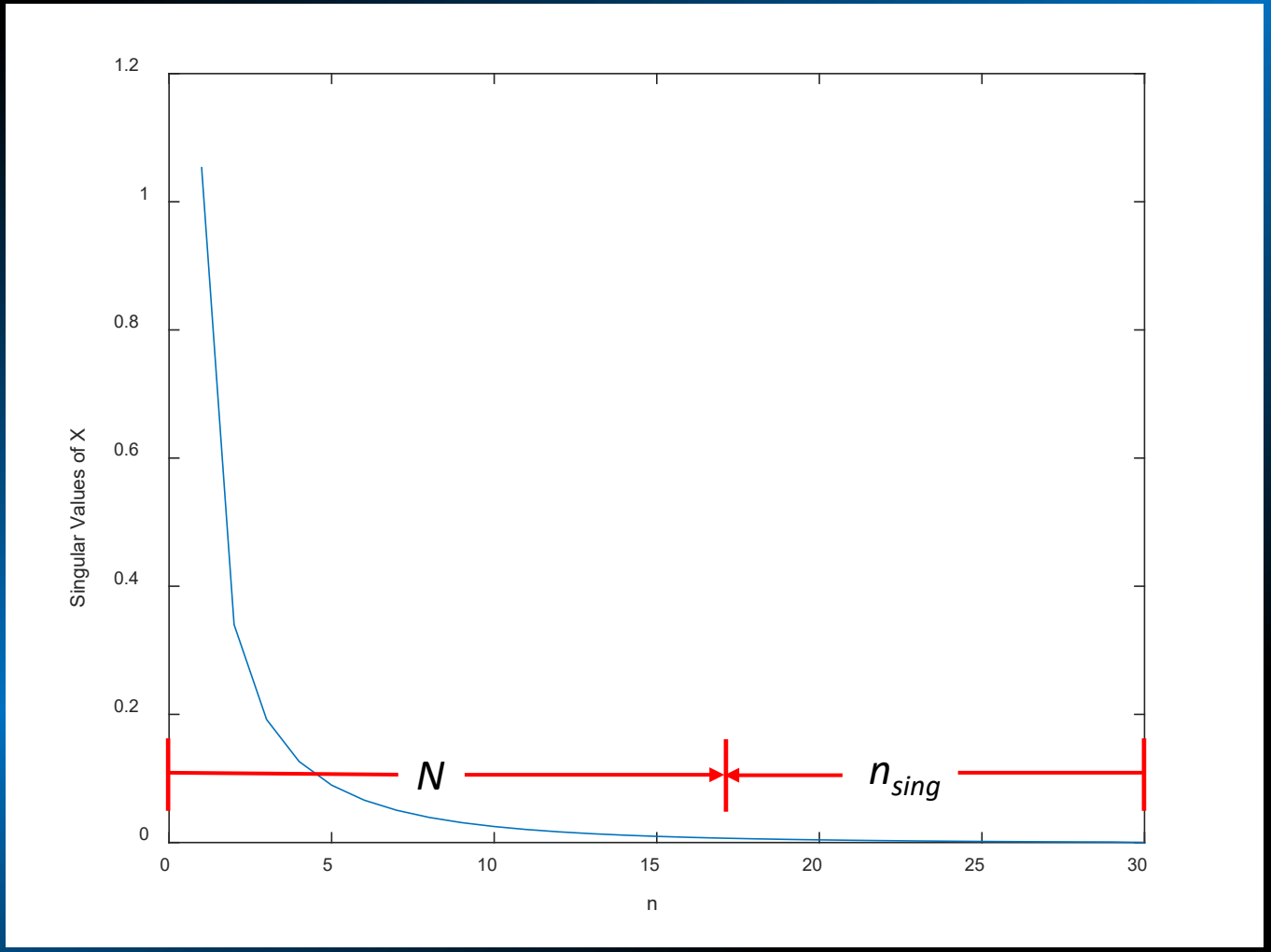
where

$$diag\left(1/w_j\right) = \begin{bmatrix} 1/w_1 & 0 & \cdots & 0 & & 0 \\ 0 & \ddots & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1/w_N & 0 & \cdots & 0 \\ \vdots & \cdots & 0 & 0 & 0 & \vdots \\ 0 & \cdots & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}$$

N is the number of *singular values* retained

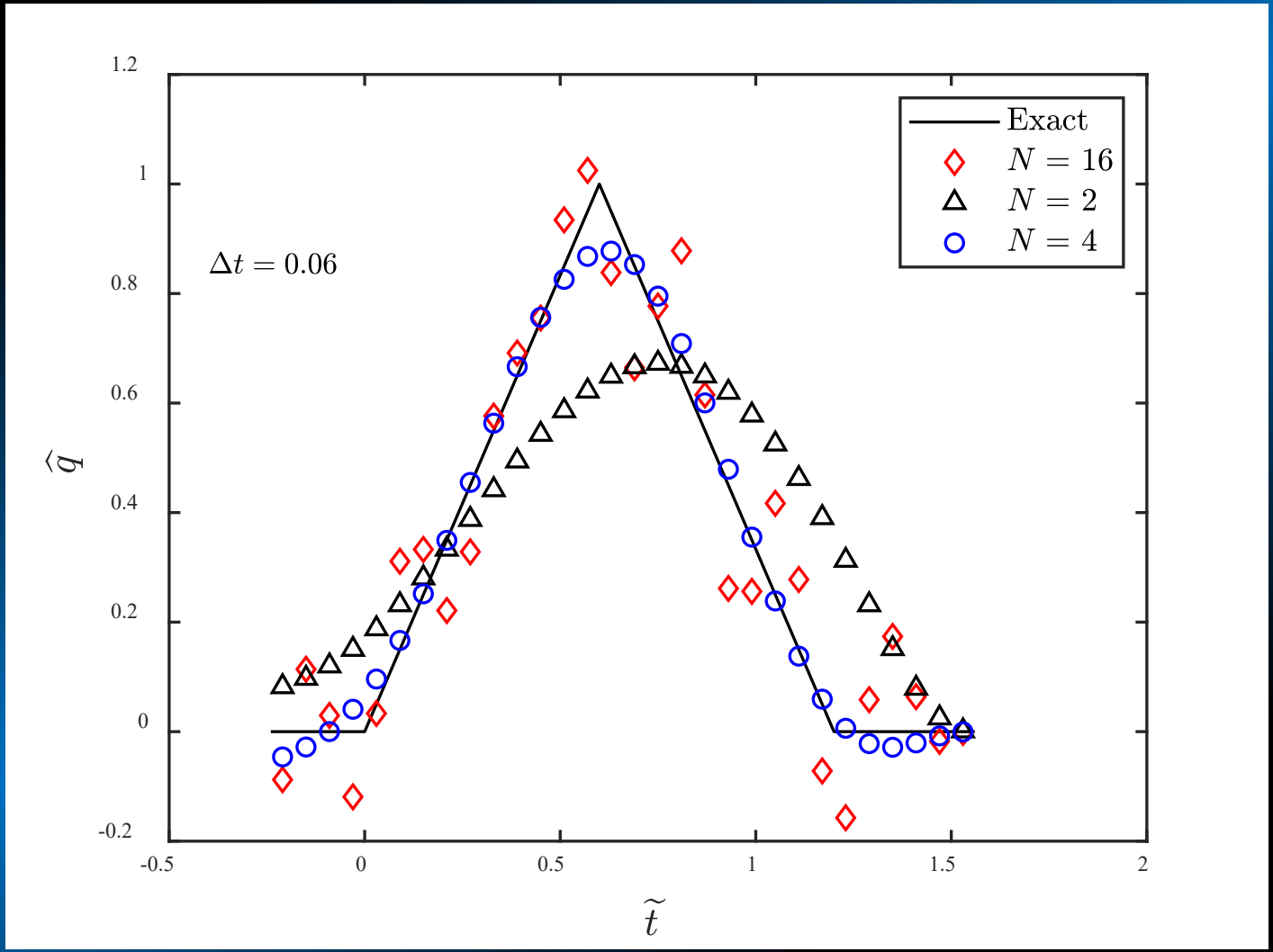
Singular Values of X

- For the X22B?0T0 problem with $\Delta t = 0.06$



N (or n_{sing}) is the regularizing parameter

TSVD - Example



Optimization of Regularization

Optimization of Regularization

- Two competing sources of error
  - Random error – due to instability of IHCP
  - Bias error – due to regularization of the method
- A compromise between these effects must be made
  - Too little regularization -> Random error dominates
  - Too much regularization -> Bias error dominates
- Some approaches
  - Morozov Discrepancy Principle
  - Minimize E(R_q)
  - L-curve

Temperatures and fluxes

- Measurements $\mathbf{Y}$

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_N \end{bmatrix} = \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_N \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_N \end{bmatrix} = \mathbf{T} + \boldsymbol{\varepsilon}$$

T are the true temperatures

ε are randomly distributed errors with standard deviation σ_y

- True, unknown, heat flux vector $\mathbf{q}$

$$\mathbf{q} = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_N \end{bmatrix}$$

Estimated q and Y

- From the IHCP solution the estimated heat flux

$$\hat{\mathbf{q}} = \mathbf{F}\mathbf{Y} = \mathbf{F}\left(\mathbf{T} + \boldsymbol{\varepsilon}\right) \qquad \mathbf{F} = \left(\mathbf{X}^T\mathbf{X} + \alpha_0\mathbf{I}\right)^{-1}\mathbf{X}^T$$

(e.g., zeroth order Tikhonov)

- Using this estimated heat flux in the measurement model (the direct problem solution) gives the "estimated measurement"

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\mathbf{q}} = \mathbf{X}\mathbf{F}\mathbf{Y} = \mathbf{X}\mathbf{F}\left(\mathbf{T} + \boldsymbol{\varepsilon}\right)$$

$$\hat{\mathbf{Y}} = \mathbf{R}\mathbf{Y}; \qquad \mathbf{R} = \mathbf{X}\mathbf{F}$$

Optimality Criteria - Temperature

- Residuals of Temperature

$$R_T = (\mathbf{Y} - \hat{\mathbf{Y}})^T (\mathbf{Y} - \hat{\mathbf{Y}})$$

- Expected value of R_T
  - With standard statistical assumptions of additive, uncorrelated errors with zero mean and known variance

True temperature

$$E(R_T) = \mathbf{T}^T (\mathbf{I} - \mathbf{R})^T (\mathbf{I} - \mathbf{R}) \mathbf{T} + \sigma_Y^2 tr((\mathbf{I} - \mathbf{R})^T (\mathbf{I} - \mathbf{R}))$$

Bias error

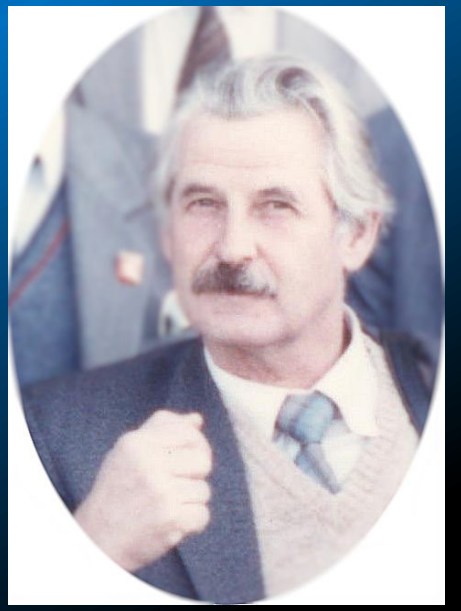
Random error

$$\mathbf{R} = \mathbf{XF}$$

Morozov Discrepancy Principle

- Choose the value of the regularization parameter so that the resulting standard error between the computed and measured data are consistent with the (known) level of noise in the data measurements

$$Mstd(R_T) = \sqrt{E(R_T)/N} = \sigma_Y$$



REGULARIZATION OF INCORRECTLY POSED PROBLEMS AND THE CHOICE OF REGULARIZATION PARAMETER*†

V. A. MOROZOV

Moscow

(*Received* 1 *March* 1965)

Optimality Criteria – Heat Flux

- Residuals of heat flux

$$R_q = (\hat{\mathbf{q}} - \mathbf{q})^T (\hat{\mathbf{q}} - \mathbf{q}) = (\mathbf{FY} - \mathbf{q})^T (\mathbf{FY} - \mathbf{q})$$

- Expected value of R_q (with standard statistical assumptions)

True heat flux

$$E(R_q) = \underbrace{[(\mathbf{FX} - \mathbf{I})\mathbf{q}]^T [(\mathbf{FX} - \mathbf{I})\mathbf{q}]}_{E_{q,bias}} + \underbrace{\sigma_Y^2 tr(\mathbf{F}^T\mathbf{F})}_{E_{q,rand}}$$

Bias error

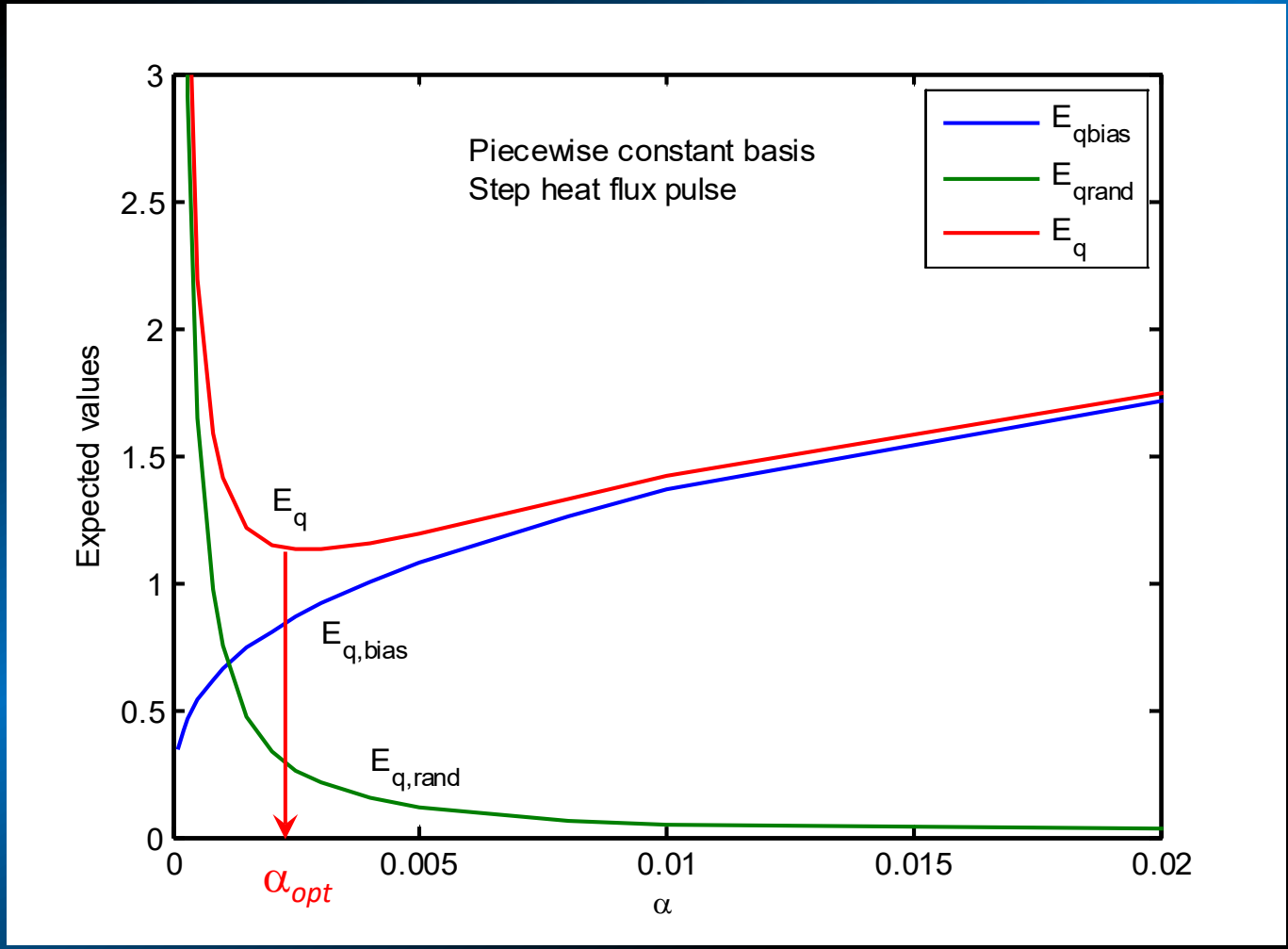
Random error

$$E_{q,bias} = [(\mathbf{FX} - \mathbf{I})\mathbf{q}]^T [(\mathbf{FX} - \mathbf{I})\mathbf{q}] = [(\mathbf{P} - \mathbf{I})\mathbf{q}]^T [(\mathbf{P} - \mathbf{I})\mathbf{q}]$$

$$E_{q,rand} = \sigma_Y^2 tr(\mathbf{F}^T\mathbf{F}) = \sigma_Y^2 tr(\mathbf{\Phi}_q); \quad \mathbf{\Phi}_q = \mathbf{F}^T\mathbf{F}$$

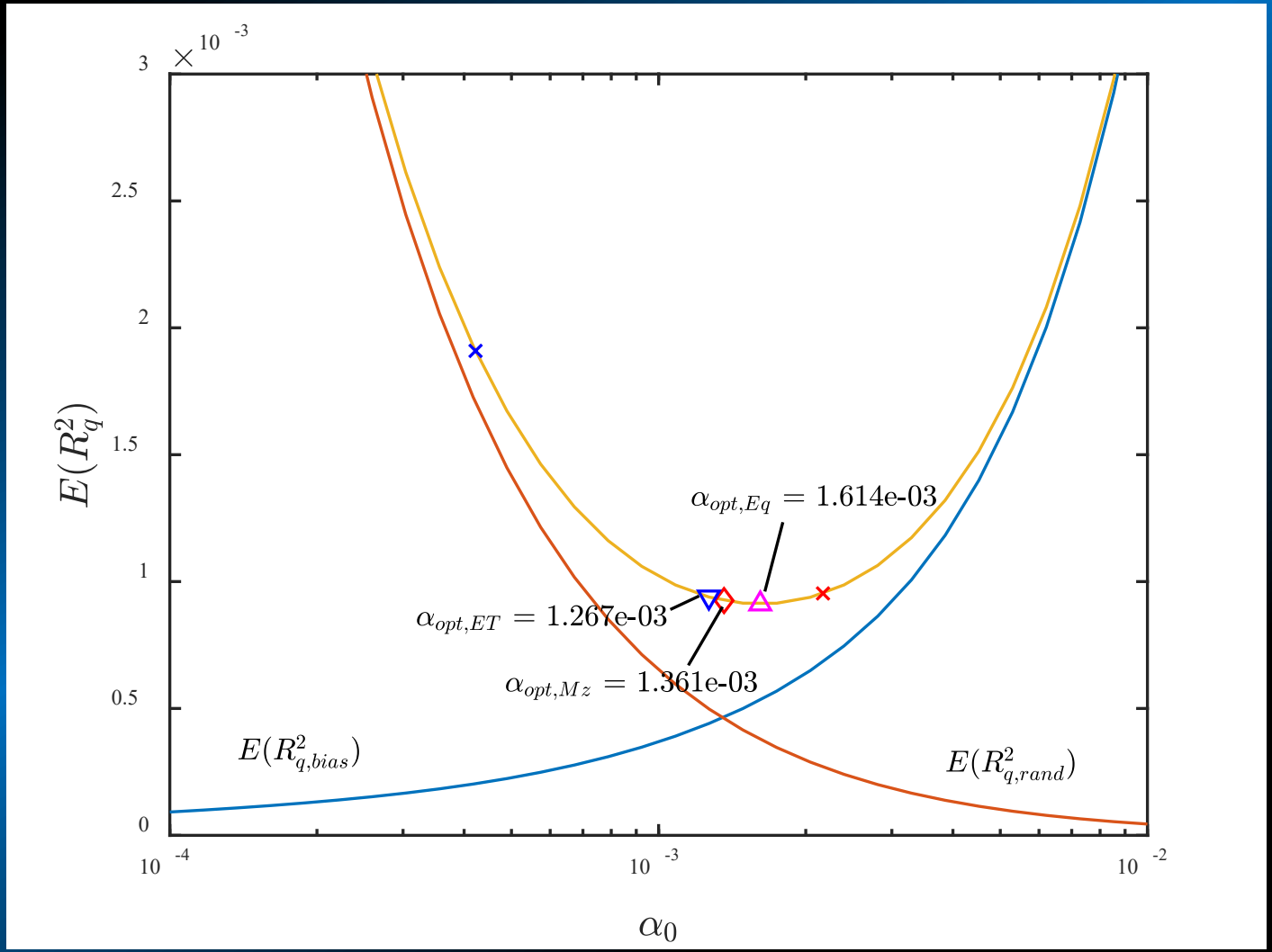
Optimal Criterion – Heat Flux

- Choose regularization to minimize E(R_q)



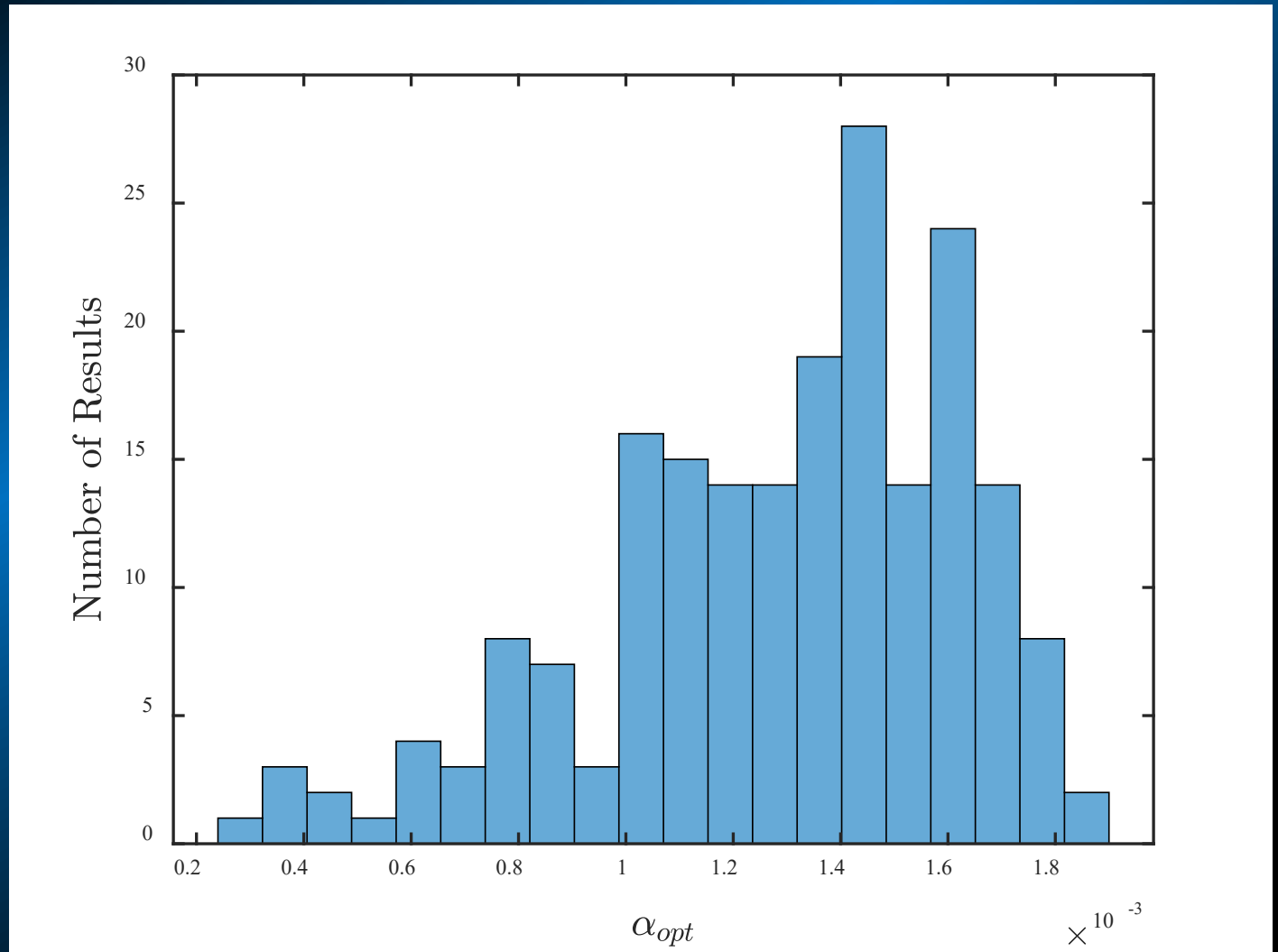
For the Example problem…

- Zeroth order Tikhonov Regularization



For the Example…

- Results from Morozov principle for 200 random sets of measurement noise



Hansen's L-curve

- Plot the norm or semi-norm of the solution versus the residual norm
- Easy to visualize trade-off between random error and bias
- Curve has characteristic "L" shape
- Optimal value for the regularization parameter is the one that puts a data point at the elbow of the curve

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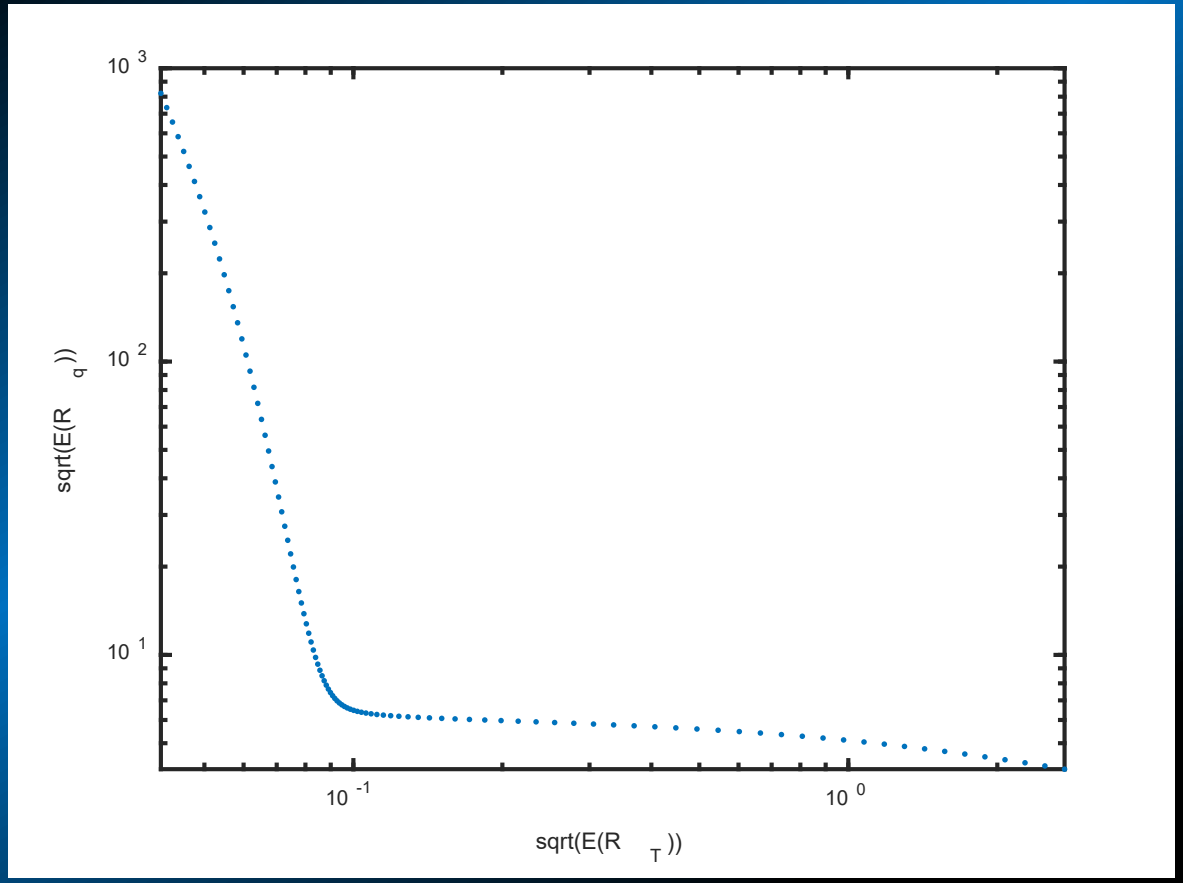
ANALYSIS OF DISCRETE ILL-POSED PROBLEMS BY MEANS OF THE L-CURVE*

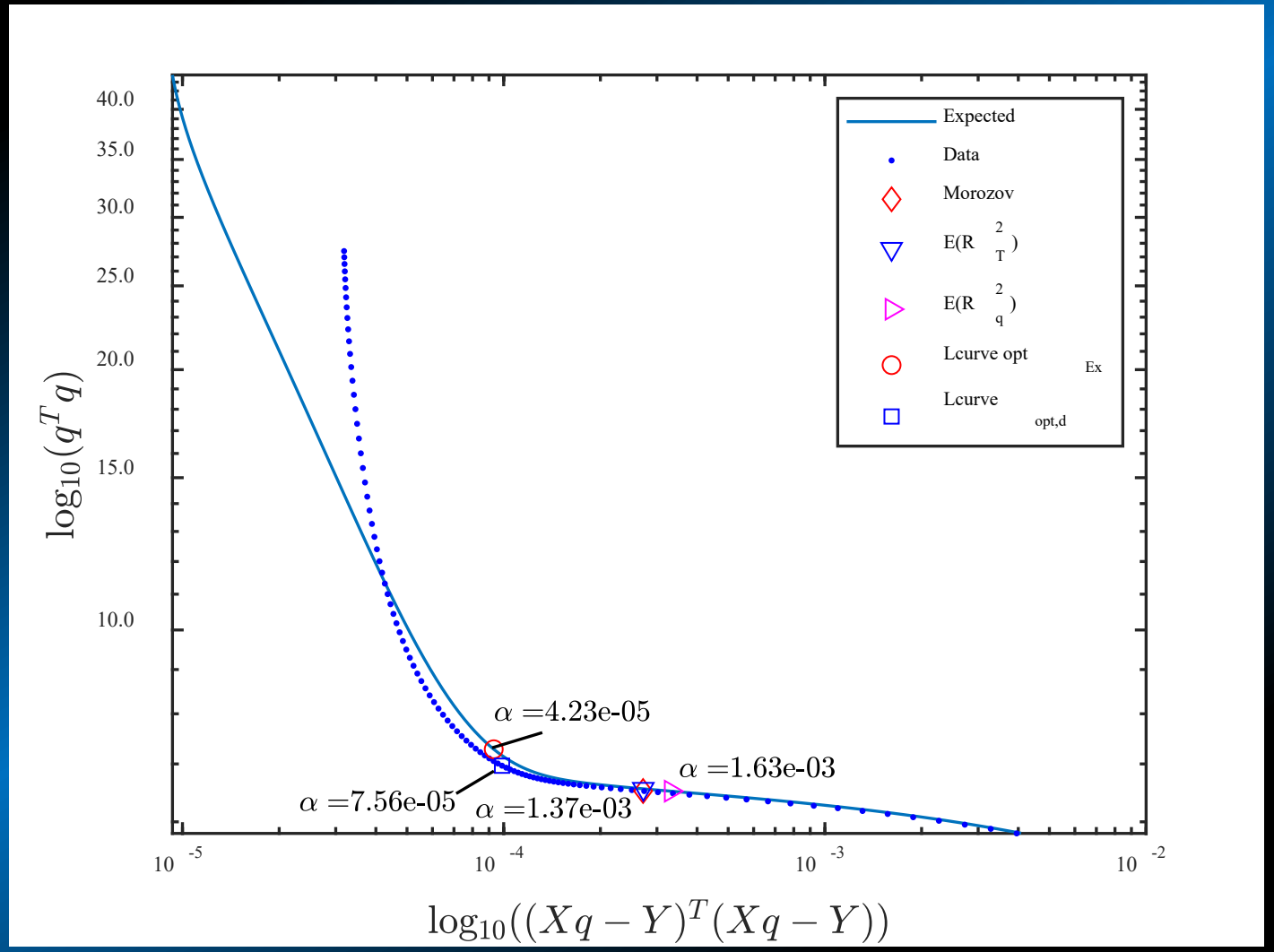
PER CHRISTIAN HANSEN†

L-curve

- Solution norm: $\|E(R_q)\|$
- Residual norm: $\|E(R_T)\|$



Criteria Comparison for Example



Summary of Optimal Regularization Methods

Method	criterion
Morozov Discrepancy Principle	Average error between estimated and measured temperatures is consistent with noise in the measured data
Minimize R_q	Strike balance between bias added and sensitivity to data noise
Hansen's L-curve	Decrease in solution norm (heat flux residuals) begins to significantly increase residual norm (temperature residuals)

Comparison of IHCP Methods

Comparison IHCP methods

- Methods
  - Function Specification (piecewise constant)
  - Tikhonov Zeroth Order
  - Tikhonov First Order
  - Conjugate Gradient (Fletcher-Reeves)
  - SVD
- Use the min E(R_q) to optimize regularization for each method
- Use
  - Step (abrupt) Heat Flux
  - Quartic (smooth) Heat Flux

Comparison: Triangular heat flux example

Method	reg. par.	$\sqrt{E\left(R_q^2\right)}$	Ranking
Func. Spec.	r = 4	0.03842	5
Tikhonov, 0th order	α_0=1.61E-3	0.02822	3
Tikhonov, 1st order	α_1=4.29E-3	0.02670	2
CG (SD)	n_{opt} = 135	0.03111	4
CG (FR)	n_{opt} = 5	0.04442	6
SVD	N = 4	0.02552	1

From Table 7.19 page 246

Summary

Summary

- IHCP Methods
  - Function Specification
  - Tikhonov
    - ✓ Zeroth Order
    - ✓ First Order
  - Conjugate Gradient
  - Singular Value Decomposition

Summary

- Optimal Regularization
  - Morozov discrepancy principle
  - Minimize Residual in Predicted Heat Flux
  - Hansen's L-curve

Summary

- Procedure given for comparing four IHCP solution methods: FS, Tikhonov, CGM, SVD
  - Triangular heat flux test case considered
  - Of methods considered, 1st order Tikhonov appears superior for filter implementation
  - but SVD also performs well

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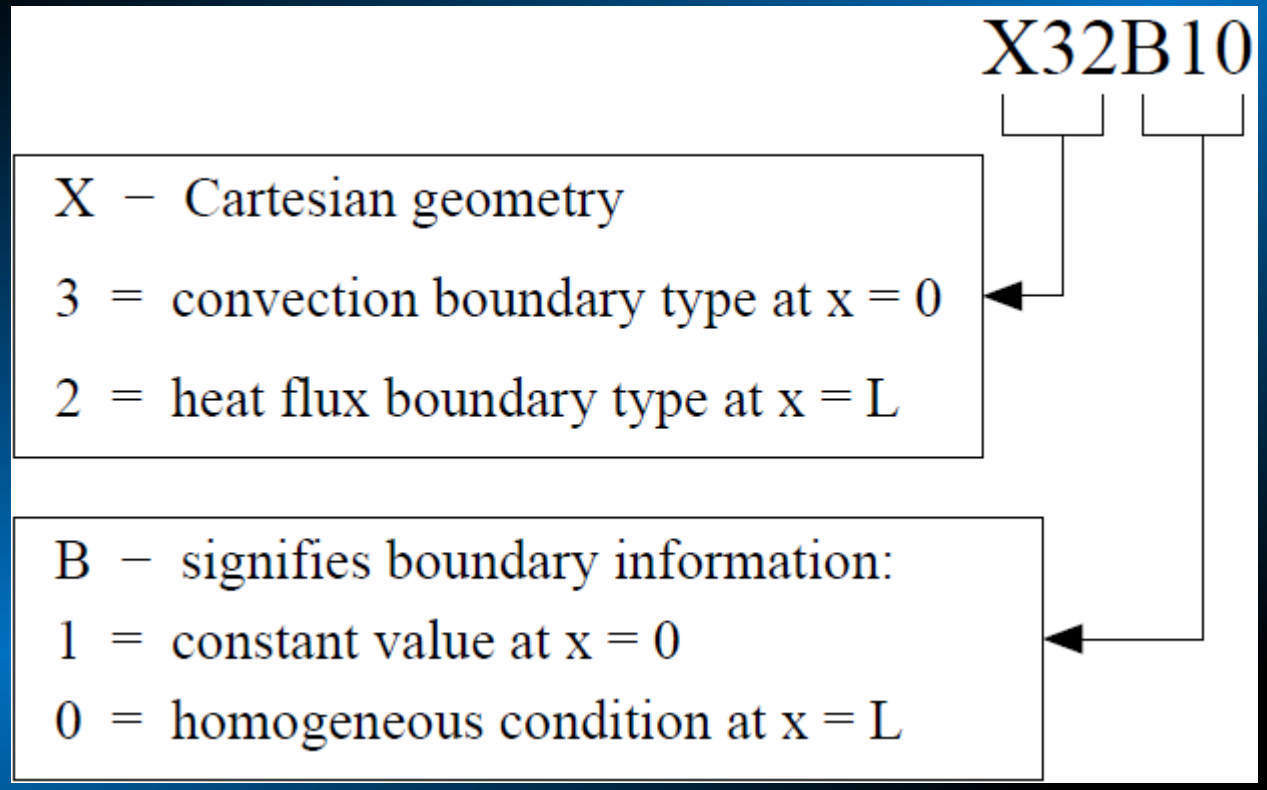
Preliminaries

Solution Numbering System

- Example: Steady-State Cartesian

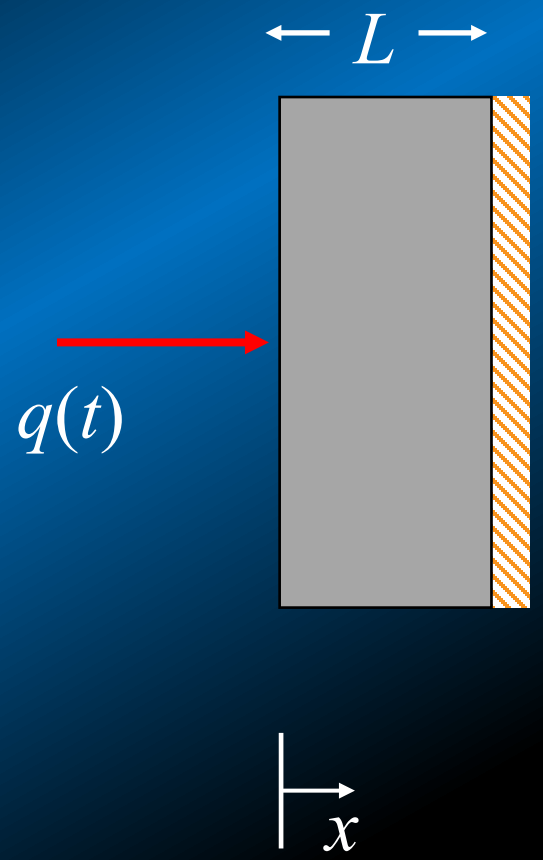


Solution Numbering System

- For the FORWARD problem:

X22B–0T0

- Cartesian
- Heat Flux at x=0
- Heat Flux at x=L
- Arbitrary Heat Flux at x=0
- Homogeneous Heat Flux at x=L
- Homogeneous Initial Temperature

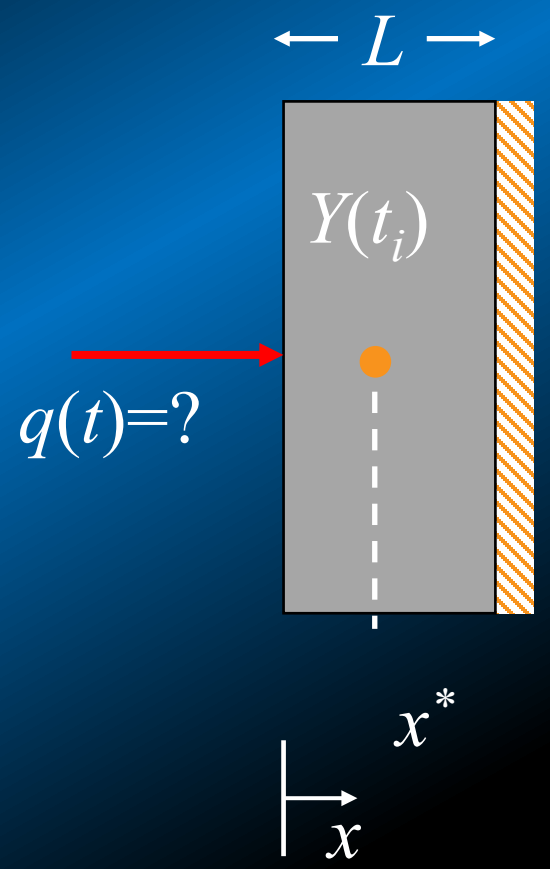


Solution Numbering System

- For the INVERSE problem:

X22B?0T0

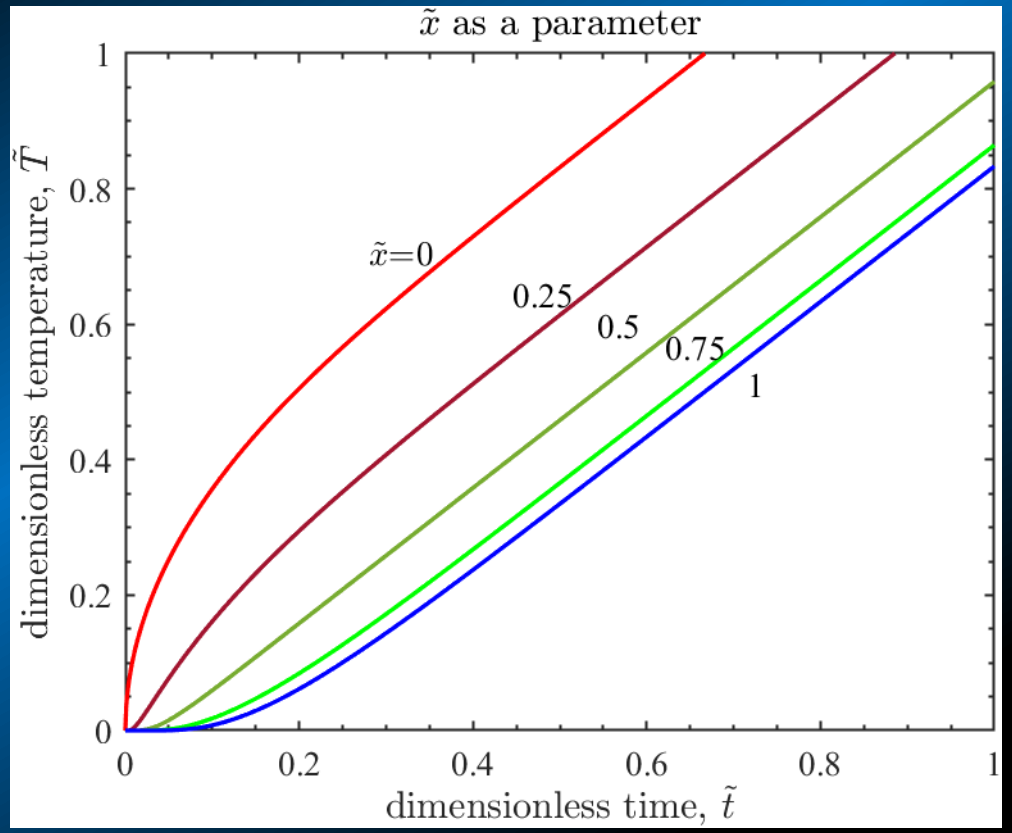
- Cartesian
- Heat Flux at x=0
- Heat Flux at x=L
- Unknown Heat Flux at x=0
- Homogeneous Heat Flux at x=L
- Homogeneous Initial Temperature



Forward Problem – Exact Solution

- For a constant heat flux at x=0 (X22B10T0)

$$T(x,t)=\frac{T_d(x,t)}{q_0 L/k}=t+\frac{1}{3}-x+\frac{x^2}{2}-\frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}e^{-n^2\pi^2 t}\cos(n\pi x)$$



Forward Problem – Exact Solution

- For linear problems, with piecewise constant heat fluxes, superposition can be used

$$\{\mathbf{T}\} = [\mathbf{X}]\{\mathbf{q}\} + T_0\{\mathbf{1}\}$$

where $\mathbf{X}$ is the *sensitivity matrix*

$$X_{ij} = \frac{\partial T_i}{\partial q_j}$$

Forward Problem – Discrete Form

- Using the exact solution for $T(x,t)$

$$X_{ij} = \frac{\partial T_i}{\partial q_j} = \begin{Bmatrix} \Delta\varphi_{i-j}, & i \geq j \\ 0, & i < j \end{Bmatrix}$$

where

$$\varphi\left(x^*, t_i\right) = t_i + \frac{1}{3} - x^* + \frac{1}{2}\left(x^*\right)^2 - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}e^{-n^2\pi^2 t}\cos\left(n\pi x^*\right)$$

$$\Delta\varphi_i = \varphi_{i+1} - \varphi_i$$

and x^* is the location of the measured temperature

Important points

- The magnitude of the entries of the **X** matrix should be as large as possible for strong sensitivity to the heat flux components
- Larger **X** matrix entries result from
  - sensors closer to the surface (smaller *x* coordinate)
  - larger time intervals between heat flux components (larger Δt)
- Example: For sensor at $x_d/L = 0.5$

0.0037	0	0	0	0
0.0194	0.0037	0	0	0
0.0267	0.0194	0.0037	0	0
0.0290	0.0267	0.0194	0.0037	0
0.0297	0.0290	0.0267	0.0194	0.0037

$$\alpha \Delta t_d / L^2 = 0.03$$

0.0231	0	0	0	0
0.0557	0.0231	0	0	0
0.0596	0.0557	0.0231	0	0
0.0600	0.0596	0.0557	0.0231	0
0.0600	0.0600	0.0596	0.0557	0.0231

$$\alpha \Delta t_d / L^2 = 0.06$$