Intro to Inverse Problems

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Motivational Example

Consider the line

$$y = f(x) = 3x + 2$$

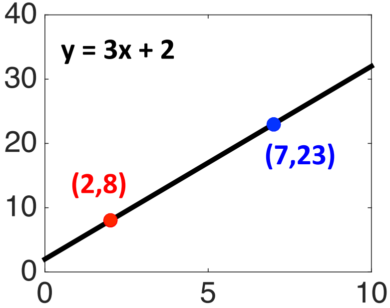
with slope $m = 3$ and y-intercept $b = 2$.

For any given x, we can compute the corresponding value of y!

$$x = 2 \quad \Rightarrow \quad y = f(2) = 8$$

$$x = 7 \quad \Rightarrow \quad y = f(7) = 23$$

$$\vdots$$



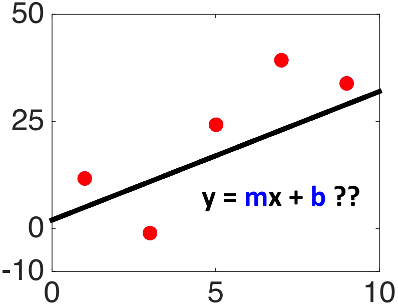
Motivational Example

Consider instead the points

$$(1, 11.72), \quad (3, -1.07), \quad (5, 24.17), \quad (7, 39.30), \quad (9, 33.89)$$

How can we find the equation of the line $\boldsymbol{y = mx + b}$ that *best fits* the given data?

Which **parameters** $\boldsymbol{m}$ and $\boldsymbol{b}$ define the line of best fit?



Motivational Example

Consider instead the points

$$(1, 11.72), \quad (3, -1.07), \quad (5, 24.17), \quad (7, 39.30), \quad (9, 33.89)$$

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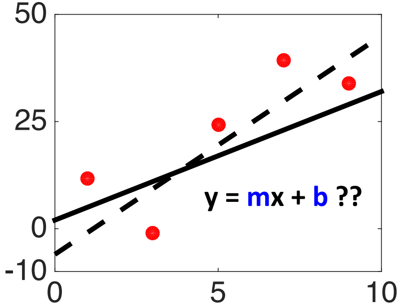

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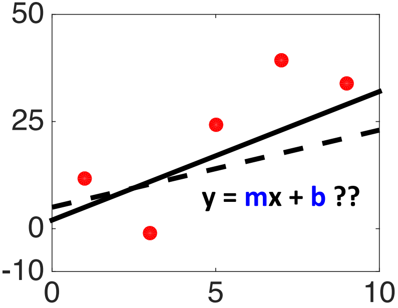
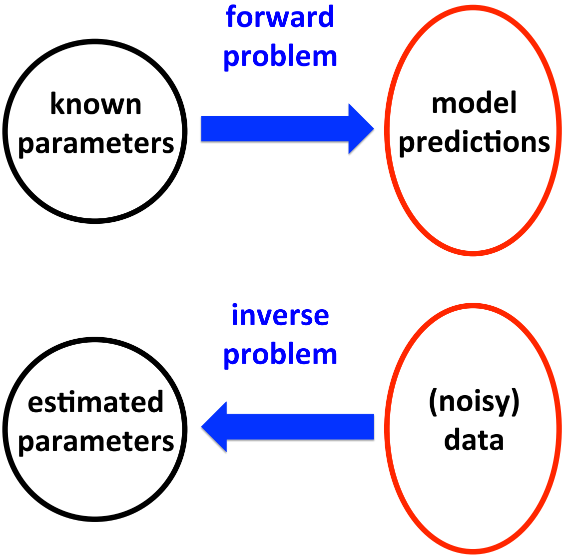


Forward vs. Inverse Problem



Forward vs. Inverse Problem

Given a map f explicitly relating two variables θ and y:

$$y = f(\theta)$$

- **Forward problem:** Compute y from known θ
- **Inverse problem:** Estimate unknown θ given y (or function of y) possibly corrupted by noise

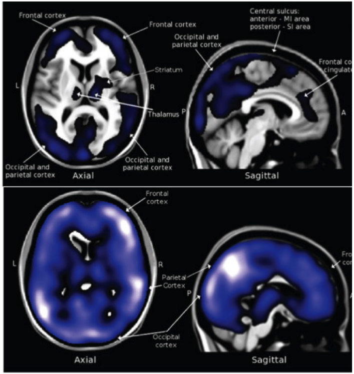
Model prediction = Forward problem

Parameter estimation = Inverse problem

Application Areas

Inverse problems arise in many fields of science and engineering

- Geophysics
- Signal processing
- Computer vision
- Machine learning
- Statistical inference
- Personalized medicine
- Medical imaging
- **Mathematical biology**



$[1\text{-}^{11}C]$-acetate PET imaging

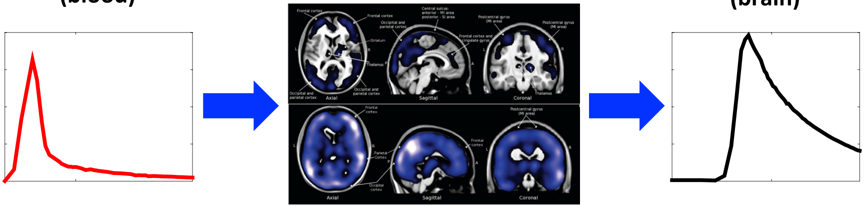
Study in vivo neurodynamics in liver disease patients using model of neurochemical kinetics and [1-^{11}C]-acetate PET measurements

- Does elevated level of ammonium in plasma primarily affect neurons or astrocytes?
- Acetate metabolized by astrocytes, not neurons!

tracer input (blood)

dynamic PET imaging

total tracer (brain)

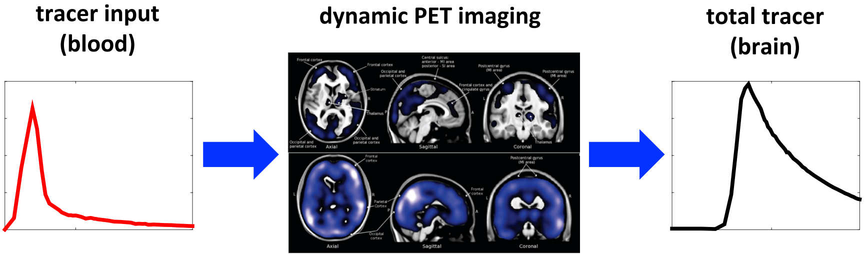


Iversen *et al.* (2009) *Gastroenterology*, 136, 863-871.

Biological Example: Acetate Metabolism in Brain

Data: 18 volunteers from 3 different groups of varying liver disease

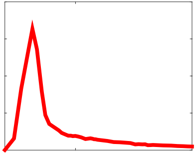
- 5 healthy control (HC)
- 7 cirrhotic liver (CL)
- 6 hepatic encephalopathy (HE)



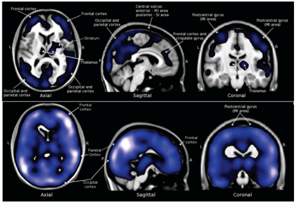
Iversen *et al.* (2009) *Gastroenterology*, 136, 863-871.

Question: Does the liver condition of the CL and HE patients significantly affect the astrocytic metabolism at the level of acetate uptake and clearance?

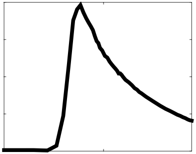
tracer input (blood)



dynamic PET imaging



total tracer (brain)



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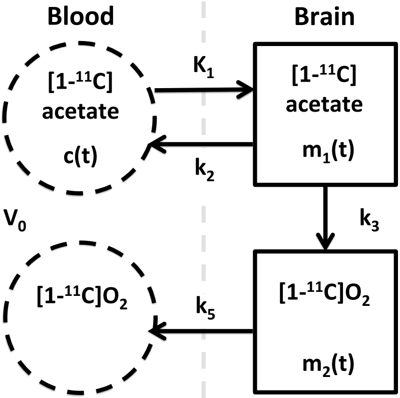


Forward model:

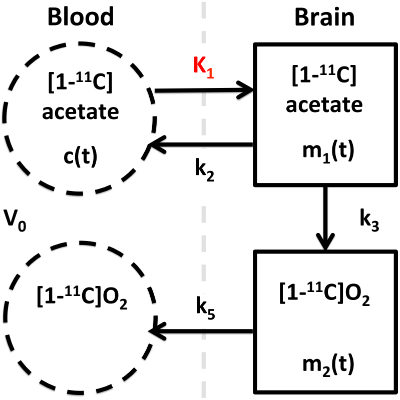
$$\begin{aligned}\frac{dm_1}{dt}(t) &= K_1 c(t) - (k_2 + k_3) m_1(t)\\ \frac{dm_2}{dt}(t) &= k_3 m_1(t) - k_5 m_2(t)\end{aligned}$$

Observation model:

$$m(t_j) = V_0 c(t_j) + m_1(t_j) + m_2(t_j)$$

Compartment model describing mass balance in the brain tissue

Example: Acetate Metabolism in Brain



Forward model:

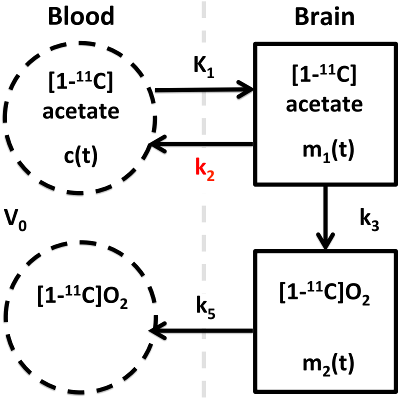
$$
\begin{aligned}
\frac{dm_1}{dt}(t) &= \boldsymbol{K_1} c(t) - (k_2 + k_3) m_1(t) \\
\frac{dm_2}{dt}(t) &= k_3 m_1(t) - k_5 m_2(t)
\end{aligned}
$$

Observation model:

$$m(t_j) = V_0 c(t_j) + m_1(t_j) + m_2(t_j)$$

$\boldsymbol{K_1}$ = clearance of tracer from blood to tissue

Example: Acetate Metabolism in Brain



Forward model:

$$\frac{dm_1}{dt}(t) = K_1 c(t) - (\boldsymbol{k_2} + k_3) m_1(t)$$

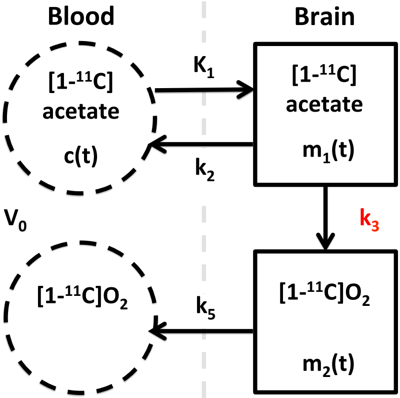
$$\frac{dm_2}{dt}(t) = k_3 m_1(t) - k_5 m_2(t)$$

Observation model:

$$m(t_j) = V_0 c(t_j) + m_1(t_j) + m_2(t_j)$$

$\boldsymbol{k_2}$, k_3, k_5 = transport rates between compartments

Example: Acetate Metabolism in Brain



Forward model:

$$\frac{dm_1}{dt}(t) = K_1 c(t) - (k_2 + \boldsymbol{k_3}) m_1(t)$$

$$\frac{dm_2}{dt}(t) = \boldsymbol{k_3} m_1(t) - k_5 m_2(t)$$

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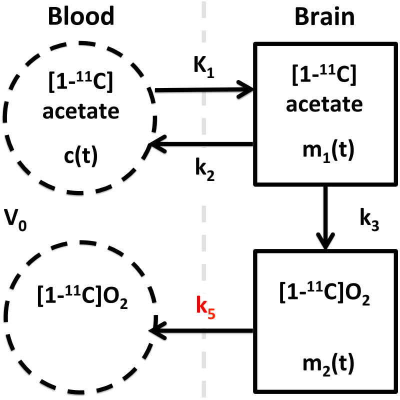
Example: Acetate Metabolism in Brain



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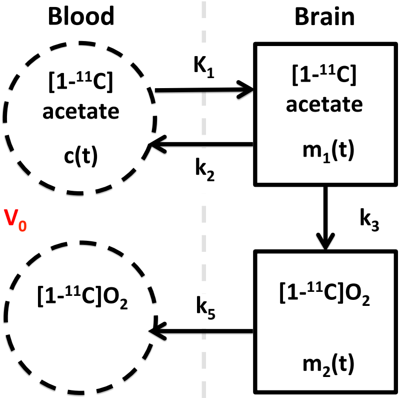
k_2, k_3, $\boldsymbol{k_5}$ = transport rates between compartments



Forward model:

$$\frac{dm_1}{dt}(t) = K_1 c(t) - (k_2 + k_3) m_1(t)$$

$$\frac{dm_2}{dt}(t) = k_3 m_1(t) - k_5 m_2(t)$$

Observation model:

$$m(t_j) = \boldsymbol{V_0} c(t_j) + m_1(t_j) + m_2(t_j)$$

$\boldsymbol{V_0}$ = virtual volume of capillary

Example: Acetate Metabolism in Brain

Forward problem

- Given: Parameters K_1, k_2, k_3, k_5, V_0 + initial conditions
- Predict: $m_1(t)$ and $m_2(t)$ for $t > 0$

Inverse problem

- Given: Noisy measurements of total acetate concentration $m(t_i)$ at times t_i, $i = 1, \ldots, n$
- Estimate: Parameters $\boldsymbol{K_1}$, $\boldsymbol{k_2}$, $\boldsymbol{k_3}$, $\boldsymbol{k_5}$, $\boldsymbol{V_0}$

Solving Inverse Problems

1. **Deterministic:** Solution is a *point estimate* of parameter values
   - Linear Least Squares
   - Nonlinear Least Squares
   - Weighted Least Squares
   - Regularization methods (e.g. Tikhonov)

2. **Bayesian:** Solution is a *distribution* of possible parameter values
   - Non-sequential sampling (e.g. MCMC)
   - Sequential filtering

Least Squares Estimation

Find parameters θ so that model $f(x_i, \theta)$ “best fits” the given data y_i

$$y_i = f(x_i, \theta) + e_i, \qquad i = 1, \dots, n$$

Solution minimizes the sum of the squares of the errors (residuals) between the model and observed data

$$e_i = y_i - f(x_i, \theta), \qquad i = 1, \dots, n$$

Optimization!

Linear Least Squares

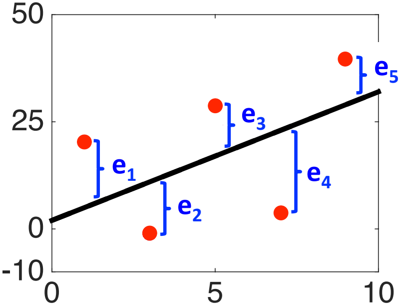
Example: Linear regression

Find the line of best fit $\hat{\boldsymbol{y}} = \boldsymbol{m}\boldsymbol{x} + \boldsymbol{b}$ to the given data!

- Given: Points (x_i, y_i), $i = 1, \ldots, n$
- Estimate: Parameters $\boldsymbol{m}$ and $\boldsymbol{b}$ that define line of best fit

Least squares approach:

Minimize the sum
of squared errors e_i!



Linear Least Squares

Inverse problem: Given the data (x_i, y_i), $i = 1, \ldots, n$, find the values of $\boldsymbol{m}$ and $\boldsymbol{b}$ that minimize the sum of the squared errors:

$$\min \sum_{i=1}^{n} e_i^2 \quad \equiv \quad \min \; S(\boldsymbol{m}, \boldsymbol{b})$$

where

$$\begin{aligned} S(m,b) \quad &:= \quad \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \quad \sum_{i=1}^{n} (y_i - \boldsymbol{m} x_i - \boldsymbol{b})^2 \end{aligned}$$

Find $\boldsymbol{m}$ and $\boldsymbol{b}$ such that $\dfrac{\partial \boldsymbol{S}}{\partial \boldsymbol{m}} = \boldsymbol{0}$ and $\dfrac{\partial \boldsymbol{S}}{\partial \boldsymbol{b}} = \boldsymbol{0}$!

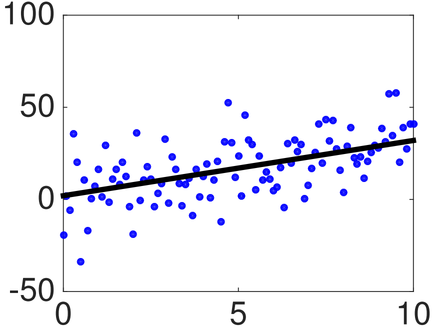
2 equations with 2 unknowns, explicitly solve for m and b:

$$\begin{aligned}\left(\sum_{i=1}^{n} x_i^2\right)\boldsymbol{m} + \left(\sum_{i=1}^{n} x_i\right)\boldsymbol{b} &= \sum_{i=1}^{n} x_i y_i \\ \left(\sum_{i=1}^{n} x_i\right)\boldsymbol{m} + n\boldsymbol{b} &= \sum_{i=1}^{n} y_i\end{aligned}$$

Least squares estimators:

$$\hat{\boldsymbol{m}} = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \quad , \quad \hat{\boldsymbol{b}} = \frac{1}{n}\left(\sum_{i=1}^{n} y_i - m\sum_{i=1}^{n} x_i\right)$$

Example: Linear regression



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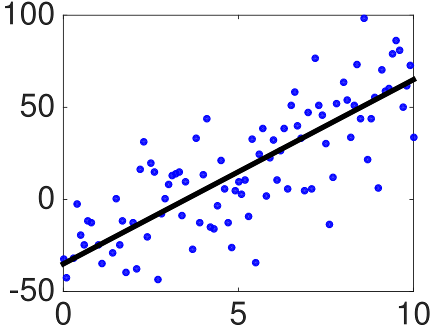
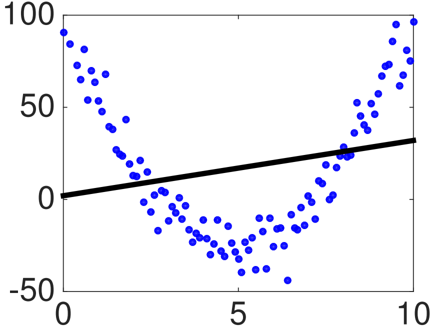
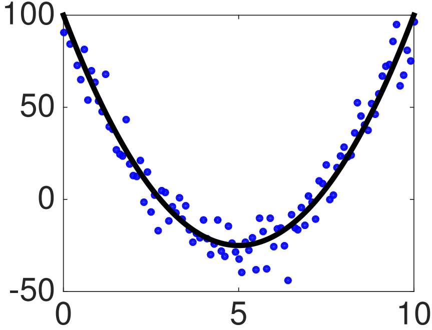


Example: Linear regression



Example: Quadratic regression



Linear Least Squares

General set-up:

$$\begin{aligned} y_i &= \theta_1 x_{i,1} + \theta_2 x_{i,2} + \cdots + \theta_p x_{i,p} + e_i, \quad i = 1, 2, \ldots, n \\ &= \mathbf{x}_i^\mathsf{T} \theta + e_i \end{aligned}$$

where

$$\mathbf{x}_i = \begin{bmatrix} x_{i,1} \\ \vdots \\ x_{i,p} \end{bmatrix} \in \mathbb{R}^p \quad \text{and} \quad \theta = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_p \end{bmatrix} \in \mathbb{R}^p$$

Note: "Linear" refers to parameters, not independent variables!

Linear Least Squares

Matrix-vector form:

$$\mathbf{y} = \mathsf{X}\theta + \mathbf{e}$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n , \qquad \mathbf{e} = \begin{bmatrix} e_1 \\ \vdots \\ e_n \end{bmatrix} \in \mathbb{R}^n ,$$

$$\mathsf{X} = \begin{bmatrix} \mathbf{x}_1^\mathsf{T} \\ \vdots \\ \mathbf{x}_n^\mathsf{T} \end{bmatrix} = \begin{bmatrix} x_{1,1} & \cdots & x_{1,p} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,p} \end{bmatrix} \in \mathbb{R}^{n \times p}$$

Inverse problem: Given the data $\mathbf{y}$, find

$$\hat{\theta} = \arg\min_{\theta} \ S(\theta)$$

where

$$S(\theta) \quad = \quad \sum_{i=1}^{n} (y_i - \mathbf{x}_i^{\mathsf{T}}\theta)^2 \quad = \quad \|\mathbf{y} - \mathsf{X}\theta\|_2^2$$

Normal equations:

$$(\mathsf{X}^{\mathsf{T}}\mathsf{X})\theta = \mathsf{X}^{\mathsf{T}}\mathbf{y}$$

Least squares estimate:

$$\hat{\theta} = (\mathsf{X}^{\mathsf{T}}\mathsf{X})^{-1}\mathsf{X}^{\mathsf{T}}\mathbf{y}$$

Nonlinear Least Squares

Modification for nonlinearities in parameters:

$$y_i = f(\mathbf{x}_i, \theta) + e_i, \quad i = 1, \ldots, n$$

where $f(\mathbf{x}_i, \theta)$ has nonlinear terms in θ

- No closed-form solution
- Must use iterative methods to estimate solution!

NLLS estimate:

$$\hat{\theta} = \arg\min_{\theta} \; S(\theta)$$

where

$$S(\theta) \;=\; \sum_{i=1}^{n} \big(y_i - f(\mathbf{x}_i, \theta)\big)^2$$

Nonlinear Least Squares

Gradient:

$$\frac{\partial S}{\partial \theta_j} = 2\sum_{i=1}^{n} e_i \frac{\partial e_i}{\partial \theta_j}, \quad j = 1, \ldots, p$$

Use iterative methods to approximate $\hat{\theta}$ that satisfies $\dfrac{\partial S}{\partial \theta_j} = 0$!

Start with initial guess θ^0, then update: At step $k+1$, the new estimate is

$$\theta^{k+1} = \theta^k + \Delta\theta$$

where the previous estimate θ^k is corrected by $\Delta\theta$

Nonlinear Least Squares

Jacobian:

$$\mathsf{J} = \left[\frac{\partial e_i}{\partial \theta_j}\right] \in \mathbb{R}^{n\times p} \ , \quad i = 1, \ldots, n, \quad j = 1, \ldots, p$$

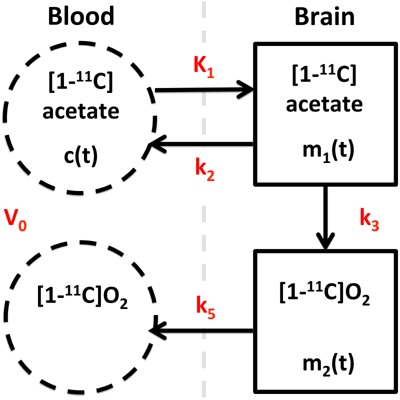
Normal equations for NLLS:

$$(\mathsf{J}^\mathsf{T}\mathsf{J})\Delta\theta = \mathsf{J}^\mathsf{T}\mathbf{e}$$

Gauss-Newton step:

$$\Delta\theta = (\mathsf{J}^\mathsf{T}\mathsf{J})^{-1}\mathsf{J}^\mathsf{T}\mathbf{e}$$

Example: Acetate Metabolism in Brain



Forward model:

$$\begin{aligned} \frac{dm_1}{dt}(t) &= K_1 c(t) - (k_2 + k_3) m_1(t) \\ \frac{dm_2}{dt}(t) &= k_3 m_1(t) - k_5 m_2(t) \end{aligned}$$

Observation model:

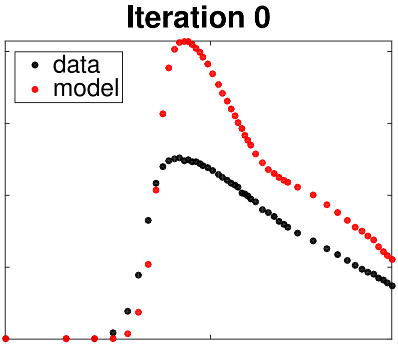
$$m(t_j) = V_0 c(t_j) + m_1(t_j) + m_2(t_j)$$

Estimate $\boldsymbol{K_1}$, $\boldsymbol{k_2}$, $\boldsymbol{k_3}$, $\boldsymbol{k_5}$, $\boldsymbol{V_0}$!

Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$
\begin{aligned}
V_0 &= 8.0000e-04 \\
K_1 &= 9.6000e-03 \\
k_2 &= 1.6000e-02 \\
k_3 &= 1.6000e-03 \\
k_5 &= 1.6000e-03
\end{aligned}
$$

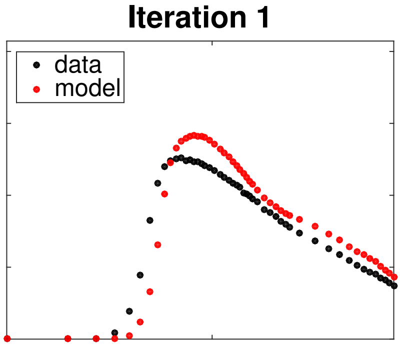


Arnold *et al.* (2015) *Mathematical Medicine & Biology*, 32 (4), 367-382

Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$V_0 = 1.0000e-04$$
$$K_1 = 6.0301e-03$$
$$k_2 = 1.2315e-02$$
$$k_3 = 1.5098e-03$$
$$k_5 = 1.5859e-03$$



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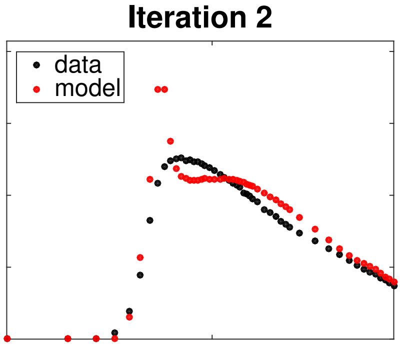
Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$
\begin{aligned}
V_0 &= 9.8783e-02 \\
K_1 &= 2.9220e-03 \\
k_2 &= 5.1900e-03 \\
k_3 &= 3.7134e-04 \\
k_5 &= 1.1363e-03
\end{aligned}
$$



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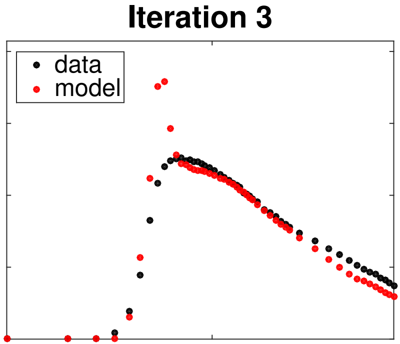
Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$
\begin{aligned}
V_0 &= 9.6125e-02 \\
K_1 &= 3.5245e-03 \\
k_2 &= 8.5702e-03 \\
k_3 &= 1.9830e-03 \\
k_5 &= 3.5272e-03
\end{aligned}
$$



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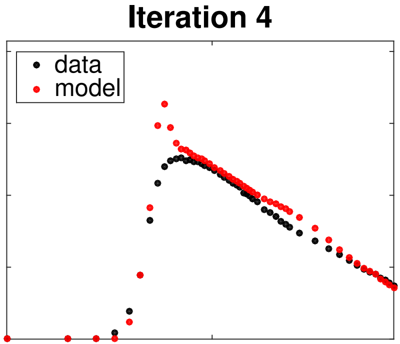
Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$\begin{aligned} V_0 &= 6.8416e-02 \\ K_1 &= 4.7904e-03 \\ k_2 &= 1.4403e-02 \\ k_3 &= 6.3611e-03 \\ k_5 &= 3.2959e-03 \end{aligned}$$



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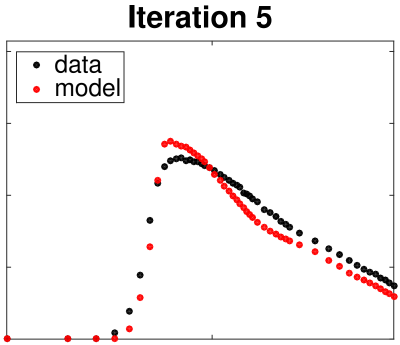
Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$\begin{aligned} V_0 &= 3.5012e-02 \\ K_1 &= 5.7135e-03 \\ k_2 &= 1.6762e-02 \\ k_3 &= 2.3035e-03 \\ k_5 &= 2.4845e-03 \end{aligned}$$



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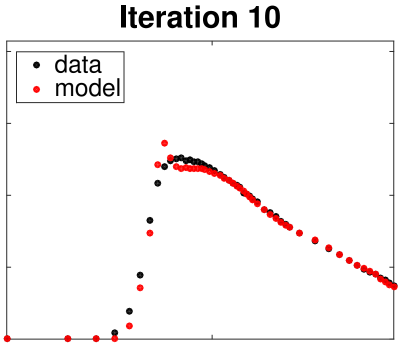
Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$
\begin{aligned}
V_0 &= 5.3690e-02\\
K_1 &= 4.1074e-03\\
k_2 &= 9.6078e-03\\
k_3 &= 1.4268e-03\\
k_5 &= 1.7815e-03
\end{aligned}
$$



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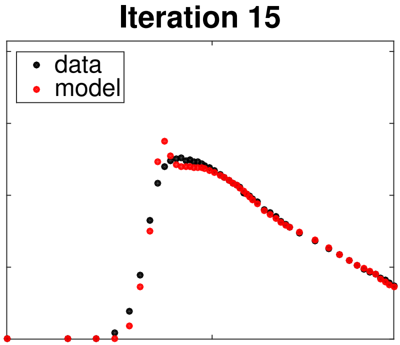
Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$
\begin{aligned}
V_0 &= 5.4292e-02 \\
K_1 &= 4.1699e-03 \\
k_2 &= 9.8703e-03 \\
k_3 &= 1.5060e-03 \\
k_5 &= 1.8212e-03
\end{aligned}
$$



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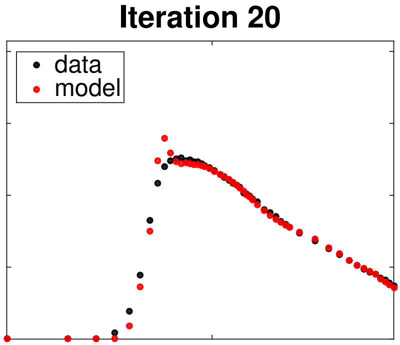
Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$V_0 = 5.3836e-02$$
$$K_1 = 4.3073e-03$$
$$k_2 = 1.0373e-02$$
$$k_3 = 1.6380e-03$$
$$k_5 = 1.8854e-03$$



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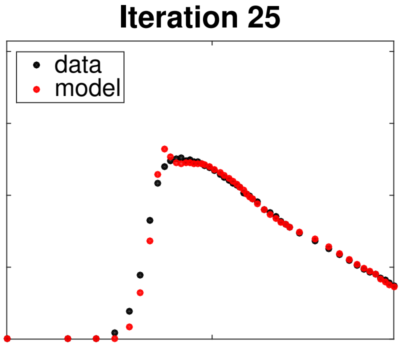
Example: Acetate Metabolism in Brain

Use NLLS to find parameter values that best fit data

$$\begin{aligned} V_0 &= 4.6091e-02 \\ K_1 &= 4.4525e-03 \\ k_2 &= 1.0555e-02 \\ k_3 &= 1.6081e-03 \\ k_5 &= 1.8802e-03 \end{aligned}$$



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Deterministic vs. Bayesian Solutions

Deterministic methods (like least squares) result in a single point estimate of parameter values

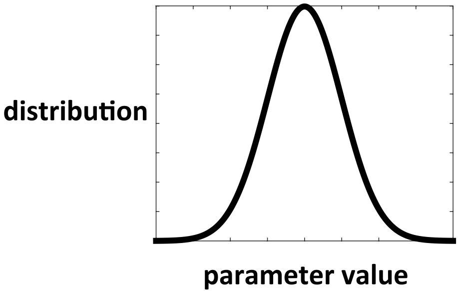
- No automatic measure of uncertainty in solution or corresponding model predictions
- Need to apply, e.g., frequentist statistics formulas

Bayesian methods (like filtering) result in a distribution of possible parameter values

- Provides natural framework for including uncertainties
- Prior information can be easily encoded
- Automatic measure of reliability in solution

Bayesian Solution

Bayesian approach to solving inverse problems involves modeling all unknown quantities as **random variables**



- Randomness described in terms of probability distributions
- Distributions convey what is known about parameter values and to what extent
- Provides a natural link between inverse problems and statistical inference

Bayesian Solution

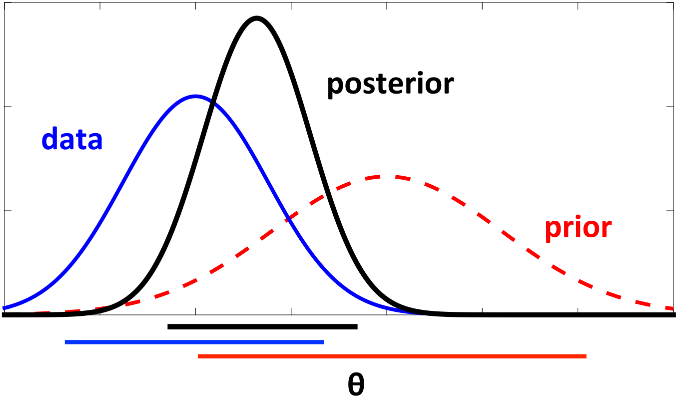
Bayes' theorem:

$$\pi(\theta \mid \mathbf{y}) \propto \pi(\mathbf{y} \mid \theta)\pi(\theta)$$

where

- $\pi(\theta \mid \mathbf{y})$ is the posterior density (solution) of parameters θ given the data $\mathbf{y}$
- $\pi(\mathbf{y} \mid \theta)$ is the likelihood of obtaining the data $\mathbf{y}$ given the parameters θ
- $\pi(\theta)$ is the prior density, encoding any known information about the parameters θ

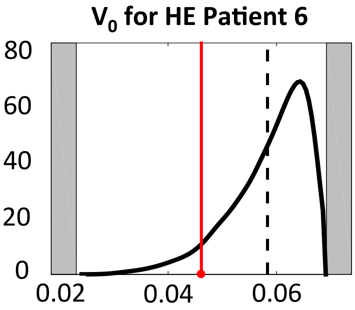
Bayesian Solution

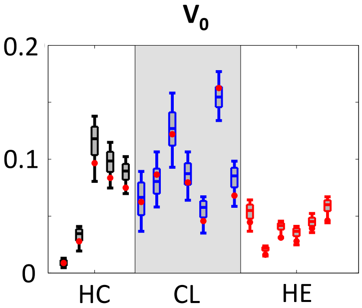


Example: Acetate Metabolism in Brain

Apply nonlinear Bayesian filter to estimate parameter distributions

- Use NLLS parameter values to inform prior!





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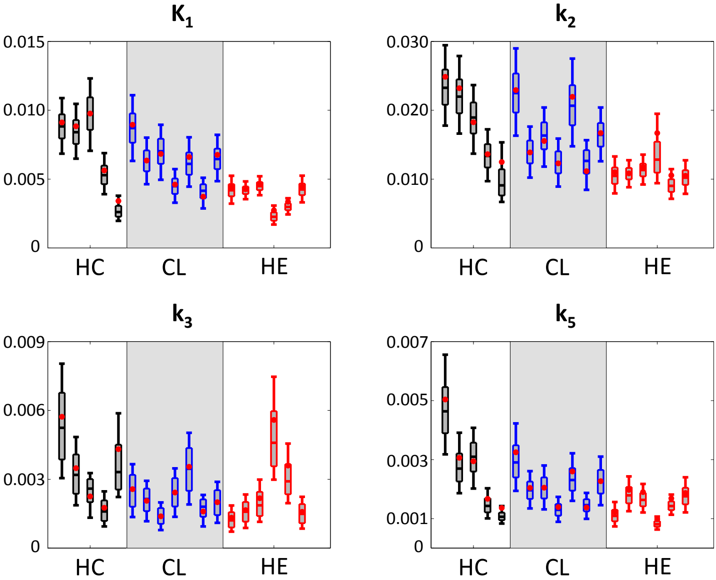
Example: Acetate Metabolism in Brain



Conclusions

Deterministic and Bayesian techniques for solving inverse problems

- Application to mathematical biology
- Not mutually exclusive – combination of techniques can be useful!

Inverse problems texts (deterministic)

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- J. P. Kaipio and E. Somersalo (2005) *Statistical and Computational Inverse Problems*. Applied Mathematical Sciences. Springer, New York.
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- A. Arnold and A. L. Lloyd (2018) An approach to periodic, time-varying parameter estimation using nonlinear filtering. Accepted, to appear in *Inverse Problems*.

Thank you!