Paremeter Estimation in Dynamical Systems

Scientific Computing for Systematic Model Building

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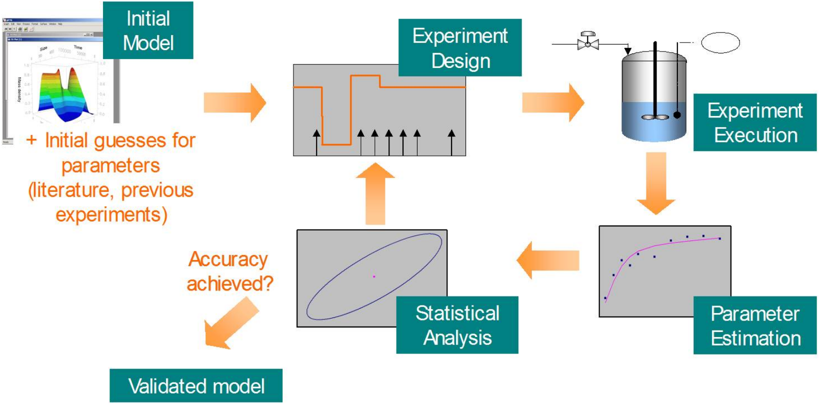
02610 Optimization and Data Fitting

Mathematical Model Building

The Model Building Cycle



Deterministic Continuous-Discrete Dynamical Model

- Ordinary Differential Equations (ODEs) and output equation

$$\begin{aligned} x(t_0) &= \hat{x}_0 \\ \frac{dx}{dt}(t) &= f(x(t), u(t), d(t), \theta) \\ y(t_k) &= g(x(t_k), \theta) \end{aligned}$$

- Reformulation

$$\begin{aligned} x(t_0) &= \hat{x}_0 \\ dx(t) &= f(x(t), u(t), d(t), \theta)dt \\ y(t_k) &= g(x(t_k), \theta) \end{aligned}$$

- Explicit Euler Discretization

$$\begin{aligned} x_0 &= \hat{x}_0 \\ x_{k+1} &= x_k + f(x_k, u_k, d_k, \theta)\Delta t = F(x_k, u_k, d_k, \theta) \\ y_k &= g(x_k, \theta) \end{aligned}$$

Stochastic Continuous-Discrete Dynamical Model

- Ordinary Differential Equations (ODEs) and output equation

$$
\begin{aligned}
x(t_0) &= \hat{x}_0 \\
dx(t) &= f(x(t), u(t), d(t), \theta)dt \\
y(t_k) &= g(x(t_k), \theta)
\end{aligned}
$$

- Stochastic Differential Equations (SDEs) and output equation

$$
\begin{aligned}
\boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
d\boldsymbol{x}(t) &= \overbrace{f(\boldsymbol{x}(t), u(t), d(t), \theta)dt}^{=\text{drift}} + \overbrace{\sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t)}^{=\text{diffusion}} & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\
\boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

- Euler-Maruyama Discretization (Explicit-Explicit)

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + f(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta t + \sigma(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta\boldsymbol{\omega}_k & \Delta\boldsymbol{\omega}_k &\sim N_{iid}(0, I\Delta t) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

- Stochastic Differential Equations (SDEs) and output equation

$$
\begin{aligned}
\boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
d\boldsymbol{x}(t) &= f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\
\boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

- Euler-Maruyama Discretization (Explicit-Explicit)

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + f(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta t + \sigma(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta\boldsymbol{\omega}_k & \Delta\boldsymbol{\omega}_k &\sim N_{iid}(0, I\Delta t) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

- Discretized system

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= F(\boldsymbol{x}_k, u_k, d_k, \boldsymbol{w}_k, \theta) & \boldsymbol{w}_k &\sim N_{iid}(0, Q) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

with

$$
\begin{aligned}
F(\boldsymbol{x}_k, u_k, d_k, \boldsymbol{w}_k, \theta) &= \boldsymbol{x}_k + f(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta t + \sigma(\boldsymbol{x}_k, u_k, d_k, \theta)\boldsymbol{w}_k \\
\boldsymbol{w}_k &= \Delta\boldsymbol{\omega}_k \sim N_{iid}(0, I\Delta t) = N_{iid}(0, Q), \; Q = I\Delta t
\end{aligned}
$$

- Stochastic Differential Equations (SDEs) and output equation

$$
\begin{aligned}
\boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
d\boldsymbol{x}(t) &= f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\
\boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

- Euler-Maruyama Discretization (Explicit-Explicit)

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + f(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta t + \sigma(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta\boldsymbol{\omega}_k & \Delta\boldsymbol{\omega}_k &\sim N_{iid}(0, I\Delta t) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

- Discretized system

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= F(\boldsymbol{x}_k, u_k, d_k, \theta) + \boldsymbol{w}_k, & \boldsymbol{w}_k &\sim N_{iid}(0, Q_k(\theta)) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R(\theta))
\end{aligned}
$$

with

$$
\begin{aligned}
F(\boldsymbol{x}_k, u_k, d_k, \boldsymbol{w}_k, \theta) &= \boldsymbol{x}_k + f(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta t \\
\boldsymbol{w}_k &= [\sigma(\boldsymbol{x}_k, u_k, d_k, \theta)\Delta\boldsymbol{\omega}_k] \sim N_{iid}(0, Q_k(\theta)) \\
Q_k(\theta) &= \sigma(\boldsymbol{x}_k, u_k, d_k, \theta)\,[I\Delta t]\,\sigma(\boldsymbol{x}_k, u_k, d_k, \theta)' \\
&= \left[\sigma(\boldsymbol{x}_k, u_k, d_k, \theta)\sigma(\boldsymbol{x}_k, u_k, d_k, \theta)'\right]\Delta t
\end{aligned}
$$

Filtering and Prediction

Extended Kalman Filter (EKF)

- Discrete-time model

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= F(\boldsymbol{x}_k, u_k, d_k, \theta) + \boldsymbol{w}_k, & \boldsymbol{w}_k &\sim N_{iid}(0, Q_k) \quad Q_k = Q_k(\theta) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R_k) \quad R_k = R(\theta)
\end{aligned}
$$

- Extended Kalman Filter Algorithm ($\hat{x}_{0|-1} = \hat{x}_0$, $P_{0|-1} = \hat{P}_0$)
  - Measurement update

$$
\begin{aligned}
\hat{y}_{k|k-1} &= g(\hat{x}_{k|k-1}, \theta) & C_k &= \frac{\partial g}{\partial x}(\hat{x}_{k|k-1}, \theta) \\
e_k &= y_k - \hat{y}_{k|k-1} & R_{e,k} &= C_k P_{k|k-1} C_k' + R_k \\
\hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_k e_k & K_k &= P_{k|k-1} C_k' R_{e,k}^{-1}
\end{aligned}
$$

$$
P_{k|k} = P_{k|k-1} - K_k R_{e,k} K_k' = (I - K_k C_k) P_{k|k-1} (I - K_k C_k)' + K_k R_k K_k'
$$

  - Time update (One-step prediction)

$$
\begin{aligned}
\hat{x}_{k+1|k} &= F(\hat{x}_{k|k}, u_k, d_k, \theta) \\
P_{k+1|k} &= A_k P_{k|k} A_k' + Q_k \qquad A_k = \frac{\partial F}{\partial x}(\hat{x}_{k|k}, u_k, d_k, \theta)
\end{aligned}
$$

Continuous-Discrete Extended Kalman Filter (CDEKF)

- Continuous-Discrete Stochastic Model

$$\begin{aligned}
\boldsymbol{x}(t_0) &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
d\boldsymbol{x}(t) &= f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) & d\boldsymbol{\omega}(t) &\sim N_{iid}(0, Idt) \\
\boldsymbol{y}(t_k) &= g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & \boldsymbol{v}(t_k) &\sim N_{iid}(0, R(\theta))
\end{aligned}$$

- Continuous-Discrete Extended Kalman Filter Algorithm ($\hat{x}_{0|-1} = \hat{x}_0$, $P_{0|-1} = \hat{P}_0$)
  - Measurement update

$$\begin{aligned}
\hat{y}_{k|k-1} &= g(\hat{x}_{k|k-1}, \theta) & C_k &= \frac{\partial g}{\partial x}(\hat{x}_{k|k-1}, \theta) \\
e_k &= y_k - \hat{y}_{k|k-1} & R_{e,k} &= C_k P_{k|k-1} C_k' + R_k \\
\hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_k e_k & K_k &= P_{k|k-1} C_k' R_{e,k}^{-1} \\
P_{k|k} &= P_{k|k-1} - K_k R_{e,k} K_k' = (I - K_k C_k) P_{k|k-1} (I - K_k C_k)' + K_k R_k K_k'
\end{aligned}$$

  - Time update - compute $\hat{x}_{k+1|k} = \hat{x}_k(t_{k+1})$ and $P_{k+1|k} = P_k(t_{k+1})$ by solving

$$\begin{aligned}
\frac{d}{dt}\hat{x}_k(t) &= f(\hat{x}_k(t), u_k, d_k, \theta) & \hat{x}_k(t_k) &= \hat{x}_{k|k} \\
\frac{d}{dt}P_k(t) &= A_k(t)P_k(t) + P_k(t)A_k(t)' + \sigma_k(t)\sigma_k(t)' & P_k(t_k) &= P_{k|k} \\
A_k(t) &= \frac{\partial f}{\partial x}(\hat{x}_k(t), u_k, d_k, \theta) \\
\sigma_k(t) &= \sigma(\hat{x}_k(t), u_k, d_k, \theta)
\end{aligned}$$

Filters and Predictors

- Discrete Stochastic Model

$$
\begin{aligned}
\boldsymbol{x}_0 &= \hat{\boldsymbol{x}}_0 & \hat{\boldsymbol{x}}_0 &\sim N(\hat{x}_0, \hat{P}_0) \\
\boldsymbol{x}_{k+1} &= F(\boldsymbol{x}_k, u_k, d_k, \theta) + \boldsymbol{w}_k, & \boldsymbol{w}_k &\sim N_{iid}(0, Q_k) \quad Q_k = Q_k(\theta) \\
\boldsymbol{y}_k &= g(\boldsymbol{x}_k, \theta) + \boldsymbol{v}_k & \boldsymbol{v}_k &\sim N_{iid}(0, R_k) \quad R_k = R(\theta)
\end{aligned}
$$

  - Extended Kalman Filter (EKF)
  - Unscented Kalman Filter (UKF)
  - Ensemble Kalman Filter (EnKF)
  - Particle Filter (PF)
- Continuous-Discrete Stochastic Model

$$
\begin{aligned}
&\boldsymbol{x}(t_0) = \hat{\boldsymbol{x}}_0 & &\hat{\boldsymbol{x}}_0 \sim N(\hat{x}_0, \hat{P}_0) \\
&d\boldsymbol{x}(t) = f(\boldsymbol{x}(t), u(t), d(t), \theta)dt + \sigma(\boldsymbol{x}(t), u(t), d(t), \theta)d\boldsymbol{\omega}(t) & &d\boldsymbol{\omega}(t) \sim N_{iid}(0, Idt) \\
&\boldsymbol{y}(t_k) = g(\boldsymbol{x}(t_k), \theta) + \boldsymbol{v}(t_k) & &\boldsymbol{v}(t_k) \sim N_{iid}(0, R(\theta))
\end{aligned}
$$

  - Continuous-Discrete Extended Kalman Filter (CDEKF)
  - Continuous-Discrete Unscented Kalman Filter (CDUKF)
  - Continuous-Discrete Ensemble Kalman Filter (CDEnKF)
  - Continuous-Discrete Particle Filter (CDPF)

Innovation

In the measurement update of the filters,
we compute the innovation and its covariance

$$e_k = e_k(\theta)$$
$$R_{e,k} = R_{e,k}(\theta)$$

The innovation is assumed to be distributed as

$$\boldsymbol{e}_k \sim N_{iid}(0, R_{e,k})$$

Statistical analysis is based on statistical tests assuming that the innovation has this distribution

Maximum-Likelihood Estimation

- Actual measurements $\{y_0, y_1, \ldots, y_{N_d}\}$
- Normally distributed independent variables

$$\boldsymbol{y}_k \sim N_{iid}(\hat{y}_k(\theta), R_k(\theta))$$

- Multivariate normal distrubtion

$$p_{y_k}(y_k; \theta) = \frac{1}{(2\pi)^{n_y/2} \left[\det R_k(\theta)\right]^{1/2}} \exp\left(-\frac{1}{2}(y_k - \hat{y}_k(\theta)) \left[R_k(\theta)\right]^{-1} (y_k - \hat{y}_k(\theta))\right)$$

$$p(\{y_k\}_{k=0}^{N_d}; \theta) = \prod_{k=0}^{N_d} p_{y_k}(y_k; \theta)$$

- Maximum Likelihood (ML) Estimation

$$\max_{\theta} \quad p(\{y_k\}_{k=0}^{N_d}; \theta) = \prod_{k=0}^{N_d} p_{y_k}(y_k; \theta)$$

- Negative log-likelihood estimation (equiv to maximum likelihood estimation)

$$L_k(\theta) = -\ln p_{y_k}(y_k; \theta) = \frac{n_y}{2} \ln(2\pi) + \frac{1}{2} \ln\left[\det R_k(\theta)\right] + \frac{1}{2}(y_k - \hat{y}_k(\theta)) \left[R_k(\theta)\right]^{-1} (y_k - \hat{y}_k(\theta))$$

$$\begin{aligned} L(\theta) &= -\ln p(\{y_k\}_{k=0}^{N_d}; \theta) = \sum_{k=0}^{N_d} L_k(\theta) \\ &= \frac{1}{2}\left(\sum_{k=0}^{N_d} \ln\left[\det R_k(\theta)\right] + \frac{1}{2}(y_k - \hat{y}_k(\theta)) \left[R_k(\theta)\right]^{-1} (y_k - \hat{y}_k(\theta))\right) + \frac{(N_d+1)n_y}{2} \ln(2\pi) \end{aligned}$$

$$\min_{\theta} \; L(\theta)$$

System Identification Methods

- Prediction-Error-Method (PEM)
  - Assume a stochastic model (discrete or continuous-discrete)
  - Compute the innovation and its covariance
    by a filter and prediction algorithm

$$
\begin{aligned}
e_k &= e_k(\theta) \\
R_{e,k} &= R_{e,k}(\theta)
\end{aligned}
$$

  - Assume that $\boldsymbol{e}_k \sim N_{iid}(0, R_{e,k})$ such that

$$
\begin{aligned}
V_{ML}(\theta) = \frac{1}{2} \sum_{k=0}^{N_d} \ln(\det R_{e,k}(\theta)) + e_k(\theta)' \left[R_{e,k}(\theta)\right]^{-1} e_k(\theta) \\
+ \frac{(N_d + 1) n_y}{2} \ln(2\pi)
\end{aligned}
$$

- Output-Error (OE)
  - Assume a deterministic model, but with measurement noise.
  - This is equivalent to a stochastic model with no process noise (diffusion) and perfectly known initial conditions. A PEM can be applied to such a system.
  - This is also know as a **simulation** model.

Parameter Estimation

$$\begin{aligned} \min_{\theta} \quad & V(\theta) \\ s.t. \quad & \theta_{\min} \leq \theta \leq \theta_{\max} \end{aligned}$$

Innovation (computed from model and data using a filter and predictor)

$$\begin{aligned} e_k(\theta) &= e_k \\ R_{e,k}(\theta) &= R_{e,k} \end{aligned}$$

Least squares (LS) objective function

$$V_{LS}(\theta) = \frac{1}{2} \sum_{k=0}^{N_d} \| e_k(\theta) \|_2^2$$

Maximum likelihood (ML) objective function

$$\begin{aligned} V_{ML}(\theta) = \frac{1}{2} \sum_{k=0}^{N_d} & \ln(\det R_{e,k}(\theta)) + e_k(\theta)' \left[R_{e,k}(\theta) \right]^{-1} e_k(\theta) \\ & + \frac{(N_d + 1) n_y}{2} \ln(2\pi) \end{aligned}$$

Maximum a posteriori (MAP) objective function

$$V_{MAP}(\theta) = V_{ML}(\theta) + \frac{1}{2} (\theta - \theta_0)' P_{\theta_0}^{-1} (\theta - \theta_0) + \frac{1}{2} \ln(\det P_{\theta_0}) + \frac{n_\theta}{2} \ln(2\pi)$$

Parameter Estimation - Bound Constrained Optimization

$$\begin{aligned} \min_{\theta} \quad & V(\theta) \\ s.t. \quad & \theta_{\min} \leq \theta \leq \theta_{\max} \end{aligned}$$

is solved by

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ s.t. \quad & l \leq x \leq u \end{aligned}$$

```
FMINCON finds a constrained minimum of a function of several variables.
FMINCON attempts to solve problems of the form:
min F(X)  subject to:  A*X  <= B, Aeq*X  = Beq (linear constraints)
X                     C(X) <= 0, Ceq(X) = 0   (nonlinear constraints)
LB <= X <= UB        (bounds)

xopt = fmincon(@fun, x0, [], [], [], [], lb, ub)
```

Parameter Estimation

Parameter Estimation

$$\min_x \; f(x)$$

- Model / prediction: $\hat{y}(x)$
- Measurement: y
- Error (residual): $e = e(x) = y - \hat{y}(x)$
- Covariance of error (residual): $R = R(x)$
- Objective function: $f(x)$
  - Least Squares (LS)

$$f(x) = \frac{1}{2} \left\| e(x) \right\|_2^2$$

  - Maximum Likelihood (ML) [negative log likelihood function]

$$f(x) = \frac{1}{2} \ln \left[\det R(x) \right] + \frac{1}{2} e(x)' R(x)^{-1} e(x)$$

- Error (residual): $e(x)$

$$e(x) = \begin{bmatrix} e_1(x) \\ \vdots \\ e_m(x) \end{bmatrix}$$

$$J(x) = \frac{\partial e}{\partial x}(x) = \begin{bmatrix} \frac{\partial e_1}{\partial x_1}(x) & \dots & \frac{\partial e_1}{\partial x_n}(x) \\ \vdots & & \vdots \\ \frac{\partial e_m}{\partial x_1}(x) & \dots & \frac{\partial e_m}{\partial x_n}(x) \end{bmatrix}$$

- Least squares (LS) objective function

$$f(x) = \frac{1}{2} \|e(x)\|_2^2$$

$$\nabla f(x) = \left[\frac{\partial e}{\partial x}(x)\right]' e(x) = J(x)' e(x)$$

$$\nabla^2 f(x) = J(x)' J(x) + \sum_i \nabla^2 e_i(x) e_i(x) \approx J(x)' J(x)$$

- error, $e(x) = y - \hat{y}(x)$, and covariance of error, $R(x)$:

$$e(x) = \begin{bmatrix} e_1(x) \\ \vdots \\ e_m(x) \end{bmatrix}$$

$$R(x) = \begin{bmatrix} R_{11}(x) & \dots & R_{1m}(x) \\ \vdots & & \vdots \\ R_{m1}(x) & \dots & R_{mm}(x) \end{bmatrix}$$

- Maximum likelihood (ML) [negative log likelihood function]

$$f(x) = \frac{1}{2} \ln\left[\det R(x)\right] + \frac{1}{2} e(x)' R(x)^{-1} e(x)$$

$$\begin{aligned} \frac{\partial f}{\partial x_i}(x) = {} & \frac{1}{2}\mathsf{tr}\left[R(x)^{-1}\frac{\partial R}{\partial x_i}(x)\right] \\ & + e(x)'R(x)^{-1}\frac{\partial e}{\partial x_i}(x) + \frac{1}{2}e(x)'R(x)^{-1}\left[\frac{\partial R}{\partial x_i}(x)\right]R(x)^{-1}e(x) \end{aligned}$$

Parameter Estimation - Objective Functions

Regression based objective functions

- ℓ_2-regression (Least Squares, LS)

$$f(x) = \frac{1}{2}\left\|e(x)\right\|_2^2 = \frac{1}{2}\left(e_1(x)^2 + e_2(x)^2 + ... + e_N(x)^2\right)$$

- ℓ_1-regression

$$f(x) = \left\|e(x)\right\|_1 = |e_1(x)| + |e_2(x)| + \ldots + |e_N(x)|$$

- ℓ_∞-regression

$$f(x) = \left\|e(x)\right\|_\infty = \max\left\{|e_1(x)|, |e_2(x)|, \ldots, |e_N(x)|\right\}$$

- ℓ_{H_γ}-regression (Huber-regression)

$$f(x) = \left\|e(x)\right\|_{H_\gamma} = \rho_\gamma(e_1(x)) + \rho_\gamma(e_2(x)) + \ldots + \rho_\gamma(e_N(x))$$

$$\rho_\gamma(e_i(x)) = \begin{cases} \frac{1}{2}e_i(x)^2 & |e_i(x)| \leq \gamma \\ \gamma\left(|e_i(x)| - \frac{1}{2}\gamma\right) & |e_i(x)| > \gamma \end{cases}$$

Parameter Estimation - Weighted Objective Functions

Weighted errors (residuals) [scaling]

$$\varepsilon(x) = We(x)$$

Optimal scaling (given the covariance, R): $W = R^{-1/2}$

- ℓ_2-regression (Least Squares, LS)

$$f(x) = \frac{1}{2}\|We(x)\|_2^2 = \frac{1}{2}\|\varepsilon(x)\|_2^2$$

- ℓ_1-regression

$$f(x) = \|We(x)\|_1 = \|\varepsilon(x)\|_1$$

- ℓ_∞-regression

$$f(x) = \|We(x)\|_\infty = \|\varepsilon(x)\|_\infty$$

- ℓ_{H_γ}-regression (Huber-regression)

$$f(x) = \|We(x)\|_{H_\gamma} = \|\varepsilon(x)\|_{H_\gamma}$$

Parameter Estimation - ML Objective Functions

Negative log-likelihood objective function for maximum likelihood (ML) estimation

- Covariance, $R = R(x)$, unknown

$$f(x) = \frac{1}{2}\ln\left[\det R(x)\right] + \frac{1}{2}e(x)'R(x)^{-1}e(x)$$

- Covariance, R, known

$$\begin{aligned} f(x) &= \frac{1}{2}\ln\left[\det R\right] + \frac{1}{2}e(x)'R^{-1}e(x) \\ &= \frac{1}{2}\ln\left[\det R\right] + \frac{1}{2}\left\|e(x)\right\|_{R^{-1}}^2 \\ &= \frac{1}{2}\ln\left[\det R\right] + \frac{1}{2}\left\|We(x)\right\|_2^2 \qquad R^{-1} = W'W \end{aligned}$$

Therefore, we can compute the ML estimate in this case by solving the weighted LS optimization problem with the objective function

$$f(x) = \frac{1}{2}\left\|We(x)\right\|_2^2 = \frac{1}{2}\left\|\varepsilon(x)\right\|_2^2$$

where the weight matrix, $W = L^{-1}$, and L is the Cholesky factor or R, i.e. $R = LL'$, such that $R^{-1} = (L^{-1})'L^{-1} = W'W$

Parameter Estimation - ML and MAP Objective Functions

$$\min_x \; f(x)$$

Negative log likelihood functions

- Maximum Likelihood (ML)

$$f(x) = \frac{1}{2}\ln\left[\det R(x)\right] + \frac{1}{2}e(x)'R(x)^{-1}e(x)$$

- Maximum a Posteriori (MAP)

$$\begin{aligned} f(x;\theta) = &\frac{1}{2}\ln\left[\det R(x)\right] + \frac{1}{2}e(x)'R(x)^{-1}e(x) \\ &+ \frac{1}{2}\ln\left[\det P(\theta)\right] + \frac{1}{2}(x - \bar{x}(\theta))'P(\theta)^{-1}(x - \bar{x}(\theta)) \end{aligned}$$

θ is a vector of hyper-parameters that can either be fixed or part of the optimization variables, i.e.

$$\min_{x,\theta} \; f(x;\theta)$$

Parameter Estimation Algorithms

Parameter Estimation Algorithms - Gradient Based

$$\min_x \ f(x)$$

Line search:

$$\min_{p_k} \phi = \frac{1}{2} p_k' H_k p_k + \nabla f(x_k)' p_k + f(x_k)$$

$$x_{k+1} = x_k + \alpha_k p_k$$

Trust region:

$$\min_{p_k} \phi = \frac{1}{2} p_k' H_k p_k + \nabla f(x_k)' p_k + f(x_k) + \frac{1}{2}\mu_k \left\| p_k \right\|_2^2$$

$$x_{k+1} = x_k + p_k$$

- Steepest descent: $H_k = I$
  Line search: $x_{k+1} = x_k - \alpha_k \nabla f(x_k)$
  Trust region: $x_{k+1} = x_k - \frac{1}{1+\mu_k} \nabla f(x_k)$
- Newton: $H_k = \nabla^2 f(x_k)$
  Line search: $x_{k+1} = x_k - \alpha_k \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k)$
  Trust region: $x_{k+1} = x_k - \left(\nabla^2 f(x_k) + \mu_k I\right)^{-1} \nabla f(x_k)$
- Quasi-Newton: H_k is an approximation to $\nabla^2 f(x_k)$
  Line search: $x_{k+1} = x_k - \alpha_k H_k^{-1} \nabla f(x_k)$
  Trust region: $x_{k+1} = x_k - (H_k + \mu_k I)^{-1} \nabla f(x_k)$

Parameter Estimation Algorithms - Least Squares

$$\min_x \; f(x) = \frac{1}{2}\|e(x)\|_2^2 = \frac{1}{2}e(x)'e(x), \qquad e(x) = y - \hat{y}(x)$$

- Gradient

$$\nabla f(x) = -\frac{\partial \hat{y}(x)}{\partial x}e(x) = -J(x)'e(x) \qquad J(x) = \frac{\partial \hat{y}(x)}{\partial x}$$

- Hessian

$$\nabla^2 f(x) = J(x)'J(x) - \sum_{i=1}^{N} \frac{\partial^2 \hat{y}_i(x)}{\partial x^2}e_i(x) = J(x)'J(x) + S(x)$$

  where

$$S(x) = -\sum_{i=1}^{N} \frac{\partial^2 \hat{y}_i(x)}{\partial x^2}e_i(x)$$

- Algorithms: $\nabla f(x_k) = -J(x_k)'e(x_k)$
  Line search: $x_{k+1} = x_k - \alpha_k H_k^{-1}\nabla f(x_k)$
  Trust region: $x_{k+1} = x_k - (H_k + \mu_k I)^{-1}\nabla f(x_k)$
  - Steepest descent: $H_k = I$
  - Newton: $H_k = \nabla^2 f(x_k) = J(x_k)'J(x_k) + S(x_k)$
  - Quasi-Newton: H_k an approximation to $\nabla^2 f(x_k)$
  - Gauss-Newton: $H_k = J(x_k)'J(x_k)$

Parameter Estimation Algorithm - Levenberg-Marquardt

$$\min_x f(x) = \frac{1}{2} \|e(x)\|_2^2 = \frac{1}{2} e(x)' e(x), \qquad e(x) = y - \hat{y}(x)$$

- Gradient

$$\nabla f(x) = -\frac{\partial \hat{y}(x)}{\partial x} e(x) = -J(x)' e(x) \qquad J(x) = \frac{\partial \hat{y}(x)}{\partial x}$$

- Hessian

$$\nabla^2 f(x) = J(x)' J(x) - \sum_{i=1}^{N} \frac{\partial^2 \hat{y}_i(x)}{\partial x^2} e_i(x) = J(x)' J(x) + S(x)$$

  where

$$S(x) = -\sum_{i=1}^{N} \frac{\partial^2 \hat{y}_i(x)}{\partial x^2} e_i(x)$$

- Levenberg-Marquardt Algorithm
  = Trust region algorithm with Gauss-Newton approximation:
  ($S(x_k) \approx 0$ such that $H_k = J(x_k)' J(x_k) \approx \nabla^2 f(x_k)$)

$$\begin{aligned} x_{k+1} &= x_k - (H_k + \mu_k I)^{-1} \nabla f(x_k) \\ &= x_k + \left(J(x_k)' J(x_k) + \mu_k I\right)^{-1} J(x_k)' e(x_k) \end{aligned}$$

Parameter Estimation - Basic Netwon Based Algorithm

The parameter estimation problem can be expressed as an unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} f(x)$$

The first order (necessary but not sufficient) optimality conditions can be expressed as

$$g(x) = \nabla f(x) = 0 \qquad g : \mathbb{R}^n \mapsto \mathbb{R}^n$$

and solved using Newton's method

$$g(x_k) + \nabla g(x_k) \Delta x_k = 0$$

This is equivalent to

$$\nabla f(x_k) + \nabla^2 f(x_k) \Delta x_k = 0$$

such that

$$\Delta x_k = -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k)$$

and

$$x_{k+1} = x_k + \Delta x_k = x_k - \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k)$$

Parameter Estimation

$$\min_{x} \quad f(x)$$

- Line-search based algorithm

$$x_{k+1} = x_k - \alpha_k H_k^{-1} \nabla f(x_k)$$

  - Newton: $H_k = \nabla^2 f(x_k)$
  - Steepest descent: $H_k = I$
  - Quasi-Newton: H_k is a rank-one approximation to $\nabla^2 f(x_k)$ based on gradient, $\nabla f(x_k)$, information

- Trust-region based algorithm

$$x_{k+1} = x_k - (H_k + \mu_k I)^{-1} \nabla f(x_k)$$

- These algorithms are gradient based algorithms, as they need gradient information, $\nabla f(x_k)$

Parameter Estimation

- Optimization problem

$$\min_{x} \quad f(x)$$

- Quadratic approximation

$$f(x_k + p_k) \approx f(x_k) + \nabla f(x_k)' p_k + \frac{1}{2} p_k' \nabla^2 f(x_k) p_k$$

- Quadratic program (QP) for search direction, p:

$$\min_{p_k} \quad \phi(p_k) = \frac{1}{2} p_k' H_k p_k + g_k' p_k + \rho_k$$

$$H_k = \nabla^2 f(x_k) \qquad g_k = \nabla f(x_k) \qquad \rho_k = f(x_k)$$

- Optimal solution to QP

$$\nabla \phi(p_k) = H_k p_k + g_k = 0 \qquad \Leftrightarrow \qquad p_k = -H_k^{-1} g_k$$

- Next iterate

$$x_{k+1} = x_k + \alpha_k p_k = x_k - \alpha_k H_k^{-1} g_k = x_k - \alpha_k \left[\nabla^2 f(x_k) \right]^{-1} \nabla f(x_k)$$

Parameter Estimation

- QP for search direction

$$\min_{p_k} \quad \phi(p_k) = \frac{1}{2}p_k' H_k p_k + g_k' p_k + \rho_k + \overbrace{\frac{1}{2}\mu_k \left\| p_k \right\|_2^2}^{\text{regularization term}}$$

- Objective function

$$\begin{aligned} \phi(p_k) &= \frac{1}{2}p_k' H_k p_k + g_k' p_k + \rho_k + \frac{1}{2}\mu_k \left\| p_k \right\|_2^2 \\ &= \frac{1}{2}p_k' H_k p_k + g_k' p_k + \rho_k + \frac{1}{2}\mu_k p_k' p_k \\ &= \frac{1}{2}p_k' \left(H_k + \mu_k I\right) p_k + g_k' p_k + \rho_k \end{aligned}$$

- Derivatives

$$\begin{aligned} \nabla \phi(p_k) &= \left(H_k + \mu_k I\right) p_k + g_k = 0 \\ \nabla^2 \phi(p_k) &= H_k + \mu_k I \end{aligned}$$

- Search direction / next iterate:

$$x_{k+1} = x_k + p_k = x_k - \left(H_k + \mu_k I\right)^{-1} g_k, \qquad g_k = \nabla f(x_k)$$

- Hessian approximations
  - Linear approximation / steepest descent variation: $H_k = I$
  - Newton: $H_k = \nabla^2 f(x_k)$
  - Quasi-Newton: H_k is an approximation to $\nabla^2 f(x_k)$

Parameter Estimation - Ways to create the trust region

- Regularized objective function

$$\min_{x} \quad \psi(x) = f(x) + \varphi_k(x)$$

  where e.g. $\varphi_k(x) = \mu_k \|x - x_k\|_2^2$
- Bound constrained estimation

$$\begin{aligned} \min_{x} \quad & f(x) \\ s.t. \quad & l \leq x \leq u \end{aligned}$$

- Constrained estimation for the trust region

$$\begin{aligned} \min_{x} \quad & f(x) \\ s.t. \quad & \|x - x_k\|_\infty \leq \Delta_k \end{aligned}$$

  is equivalent to bound constrained optimization

$$\begin{aligned} \min_{x} \quad & f(x) \\ s.t. \quad & x_k - \Delta_k e \leq x \leq x_k + \Delta_k e \end{aligned}$$

Regularization

Regularization

- Regularized optimization problem

$$\min_x \quad \psi(x) = \phi(x) + \varphi(x)$$
$$\min_x \quad \psi(x) = \phi(x) + \lambda\varphi(x)$$
$$\min_x \quad \psi(x) = \alpha\phi(x) + (1-\alpha)\varphi(x)$$

- Prediction, error and covariance

$$\hat{y} = \hat{y}(x), \qquad e(x) = y - \hat{y}(x), \qquad R = R(x)$$

- $\phi(x)$ is a function describing the fit to data

$$\phi(x) = \frac{1}{2}\left\|e(x)\right\|_2^2$$
$$\phi(x) = \frac{1}{2}\left\|W_e e(x)\right\|_2^2$$
$$\phi(x) = \frac{1}{2}\ln\left[\det R(x)\right] + \frac{1}{2}e(x)'R(x)^{-1}e(x)$$

- $\varphi(x)$ is a function describing the regularity of the solution

$$\varphi(x) = \frac{1}{2}\left\|x\right\|_2^2 \qquad \varphi(x) = \frac{1}{2}\left\|x - \bar{x}\right\|_2^2$$
$$\varphi(x) = \frac{1}{2}\left\|W_x x\right\|_2^2 \qquad \varphi(x) = \frac{1}{2}\left\|W_x(x - \bar{x})\right\|_2^2$$
$$\varphi(x) = \frac{1}{2}\ln\left[\det P\right] + \frac{1}{2}x'P^{-1}x \qquad \varphi(x) = \frac{1}{2}\ln\left[\det P\right] + \frac{1}{2}(x-\bar{x})'P^{-1}(x-\bar{x})$$

Regularization Examples

$$x = \left[x_1;\, x_2;\, \ldots;\, x_n\right], \quad x_0 = 0, \quad x_{n+1} = 0$$

- Position, x_k:

$$\varphi(x) = \frac{1}{2}\sum_{k=0}^{n+1} \|x_k\|_2^2 = \frac{1}{2}\sum_{k=1}^{n} \|x_k\|_2^2 = \frac{1}{2}\|x\|_2^2$$

- Rate, $\Delta x_k = x_k - x_{k-1}$:

$$\varphi(x) = \sum_{k=1}^{n+1} \|\Delta x_k\|_2^2 = \frac{1}{2}\|\Lambda_n x\|_2^2 \quad \Lambda_{n=4} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

- Acceleration, $\Delta^2 x_k = x_{k+1} - 2x_k + x_{k-1}$

$$\varphi(x) = \frac{1}{2}\sum_{k=1}^{n} \left\|\Delta^2 x_k\right\|_2^2 = \frac{1}{2}\left\|\Lambda_n^2 x\right\|_2^2 \quad \Lambda_{n=4}^2 = \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix}$$

Regularization terms

- Quadratic regularization terms, $\varphi(x) = \frac{1}{2}x'Hx$:

$$\begin{aligned}
\varphi(x) &= \frac{1}{2}\left\|x\right\|_2^2 = \frac{1}{2}x'x \\
&= \frac{1}{2}x'Hx && H = I \\
\varphi(x) &= \frac{1}{2}\left\|W_x x\right\|_2^2 = \frac{1}{2}(W_x x)'(W_x x) = \frac{1}{2}x'\left(W_x' W_x\right)x \\
&= \frac{1}{2}x'Hx && H = W_x' W_x
\end{aligned}$$

- Linear-quadratic regularization terms, $\varphi(x) = \frac{1}{2}x'Hx + g'x + \rho$:

$$\begin{aligned}
\varphi(x) &= \frac{1}{2}\left\|x - \bar{x}\right\|_2^2 = \frac{1}{2}(x - \bar{x})'(x - \bar{x}) = \frac{1}{2}x'x - (\bar{x})'x + \frac{1}{2}\bar{x}'\bar{x} \\
&= \frac{1}{2}x'Hx + g'x + \rho, \quad H = I, \quad g = -\bar{x}, \quad \rho = \frac{1}{2}\bar{x}'\bar{x} \\
\varphi(x) &= \frac{1}{2}\left\|W_x\left(x - \bar{x}\right)\right\|_2^2 = \frac{1}{2}(W_x(x - \bar{x}))'(W_x(x - \bar{x})) \\
&= \frac{1}{2}x'\left(W_x' W_x\right)x - \left(W_x' W_x \bar{x}\right)'x + \frac{1}{2}\bar{x}'W_x' W_x \bar{x} \\
&= \frac{1}{2}x'Hx + gx + \rho, \quad H = W_x' W_x, \quad g = -W_x' W_x \bar{x}, \quad \rho = \frac{1}{2}\bar{x}'W_x' W_x \bar{x}
\end{aligned}$$

Regularization terms - gradients and Hessians

- Quadratic regularization term

$$\begin{aligned}
\varphi(x) &= \frac{1}{2}x'Hx \\
\nabla\varphi(x) &= Hx \\
\nabla^2\varphi(x) &= H
\end{aligned}$$

- Linear-quadratic regularization term

$$\begin{aligned}
\varphi(x) &= \frac{1}{2}x'Hx + g'x + \rho \\
\nabla\varphi(x) &= Hx + g \\
\nabla^2\varphi(x) &= H
\end{aligned}$$