Mathematical Modeling

## Chapter 1

Difference equation model  $\Delta a_n = a_{n+1} - a_n = f(a_n)$ . The least-squares method for parameter estimation. Examples: Biomass growth, drug decay. Equilibrium value (EV): find a such that f(a) = a. For  $a_{n+1} = ra_n + b \ (r \neq 1)$ , the EV  $a = \frac{b}{1-r}$ . Systems of difference equations, equilibrium values. Examples: rental car company.

## Chapter 3

Model fitting (curve may not meet the points) vs interpolation (curve goes through all points).

Chebeshev criterion: minimize max error.

Least-squares criterion: minimize sum of squared er-

**Applying least-squares:** The error function

$$S(p_1, \dots, p_k) = \sum_{i=1}^{m} (y_i - f(x_i; p_1, \dots, p_k))^2$$

To mimize S:

$$\frac{\partial S}{\partial p_j} = -2\sum_{i=1}^m (y_i - f(x_i; p_1, \dots, p_k)) \frac{\partial f}{\partial p_j} = 0$$

Examples: f(x; a, b) = ax + b, f(x; a, b) = ag(x) + b $bh(x), f(x; a, b) = be^{ax}.$ 

## Chapter 4

One-term models: g(y) = af(x) + b. Find a, b using the least-squares.

High-order polynomial models: use Lagrangian form

$$P(x) = y_0 L_0(x) + y_1 L_1(x) + \dots + y_n L_n(x)$$

where the Lagrangian basis

$$L_k(x) = \prod_{i=0, i \neq k}^n \frac{x - x_i}{x_k - x_i}$$

satisfies  $L_k(x_k) = 1$  and  $L_k(x_j) = 0$  for  $j \neq k$ .

Low-order polynomial models by constructing difference tables.

Cubic splines: piecewise cubic polynomials connecting data points  $\{(x_i, y_i)\}_{i=0}^n$ , ensuring continuous first and second derivatives.

Natural boundary condition: second derivatives at endpoints are zero:  $S''(x_0) = S''(x_n) = 0$ .

#### Chapter 7

**Linear programming** problem (standard form):

$$\max/\min \sum_{i=1}^{n} c_i x_i$$
s.t. 
$$\sum_{i=1}^{n} g_{ji} x_i \le b_j, \quad j = 1, \dots, m$$

where  $x_1, \dots, x_n \geq 0$ .

Simplex method: initialization, optimality test, feasibility test, pivot.

## Chapter 13

Unconstrained optimization:

$$\max/\min \ f(x_1, \cdots, x_n)$$

Optimality conditions:  $f_{x_1} = \cdots = f_{x_n} = 0$ . Use Hessian matrix to determine local max/min. Constrained optimization:

max 
$$f(x_1, \dots, x_n)$$
  
s.t.  $g(x_1, \dots, x_n) = 0, \quad h(x_1, \dots, x_n) \ge 0$ 

Use Lagrange multiplier  $L = f + \lambda g + \mu h$ . Optimality conditions:

$$L_{x_1} = \dots = L_{x_n} = 0, \quad L_{\lambda} = g = 0$$

plus the KKT conditions:

$$L_{\mu} = h \ge 0, \quad \mu \ge 0, \quad \mu L_{\mu} = 0.$$

Minimization problem and inequality constraints in the form of  $h(x_1, \dots, x_n) \leq 0$ : conver it to the above

Sensitivity analysis: how the optimal solution changes when the parameters change.

Gradient method:

$$x_{k+1} = x_k \pm \lambda_k f_x(x_k, y_k), \quad y_{k+1} = y_k \pm \lambda_k f_y(x_k, y_k)$$

#### Chapter 8

Graph G = (V, E). Directed and undirected edges. Shortest path problem: Dijkstra's algorithm, dynamic programming.

Example: equipment replacement cost.

Maximum flow problem: Ford and Fulkerson algo-

Examples: assignment problem, matrix 0-1 problem.

#### Chapter 11

Differential equation model  $\frac{dy}{dx} = g(x, y)$ . Solve the model via **separation of variables**. Examples: population models  $\frac{dP}{dt} = kP$  and  $\frac{dP}{dt} = kP$ rP(M-P).

Equilibrium point (EP) of  $\frac{dy}{dx} = f(y)$ :  $f(y^*) = 0$ .

Phase lines: analyze signs of  $\frac{dy}{dx}$  and  $\frac{d^2y}{dx^2}$ .

Stability of EP via phase lines.

Euler's method for numerical solutions:

$$y_{n+1} = y_n + g(x_n, y_n) \Delta x$$

Parameter estimation using the least-squares method.

# Chapter 12

System of differential equations:

$$\frac{dx}{dt} = f(x, y), \quad \frac{dy}{dt} = g(x, y)$$

Equilibrium point (EP):  $f(x^*,y^*)=g(x^*,y^*)=0$ . Graphical analysis in 2D: analyze signs of  $\frac{dx}{dt},\frac{dy}{dt}$ . Stability of EP: linearization and analysis on eigenvalues of the Jacobian matrix. Euler's method for numerical solutions. *Examples*: competitive hunter model, predator-prey model.