Model Calibration by Optimization Methods

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Model Calibration

- Select model parameters to verify calibration conditions
- To find parameters minimized difference between prediction and data
- As a view of inverse prob.
- As a view of optimization prob.

Optimization Methods

The calibration procedure can be interpreted as an optimization problem of the form

$$\begin{aligned} \min_{x \in \mathcal{X}} f(x) \quad , \quad & \mathcal{X} \subseteq \mathbb{R}^n \\ \boldsymbol{x} \quad = \quad & (x_1, x_2, ..., x_n)' \end{aligned} \tag{1}$$

In general, x is not free and has some restrictions, such as $\sigma_{x_i} \geqslant 0$, wlog, we always do the optimization problem as follows:

$$\begin{aligned} & \min_{x} f(x) \\ s.j. \quad g_i(x) \quad & \leqslant \quad 0, \quad \text{for } i = 1, 2, ..., m \\ h_j(x) \quad & = \quad 0, \quad \text{for } j = 1, 2, ..., p \\ l.b_k \leqslant x_k \quad & \leqslant \quad u.b_k, \text{for } k = 1, 2, ..., n \end{aligned} \tag{2}$$

Simulated Annealing

Q: Why Simulated Annealing ?

A: For most standard strategies:

1. Most minimization (maximization) strategies work to find the nearest local minimum.

2. Generate trial point based on current estimates

3. Evaluate function at proposed location

4. Accept new value if it improves solution

Simulated Annealing

- Inspired from process of forging iron
- Annealing refers to the fast heating of a metal and then cooling it slowly
- First proposed by Metropolis(1953[3])
  - Monte-Carlo methods
  - $P = (-\Delta E/kT)$
- Kirkpatrick et al. (1982[2]) later improved the SA method applied optimization problems

Simulated Annealing

- A move is selected at random and then decides whether to accept it.
- In SA better moves are always accepted. Worse moves are not.
- The probability of accepting a worse state is a function of both the temperature of the system and the change in the cost function
- As the temperature decreases, the probability of accepting worse moves decreases
- If T=0, no worse moves are accepted (i.e. hill climbing)

Climbing Mountains

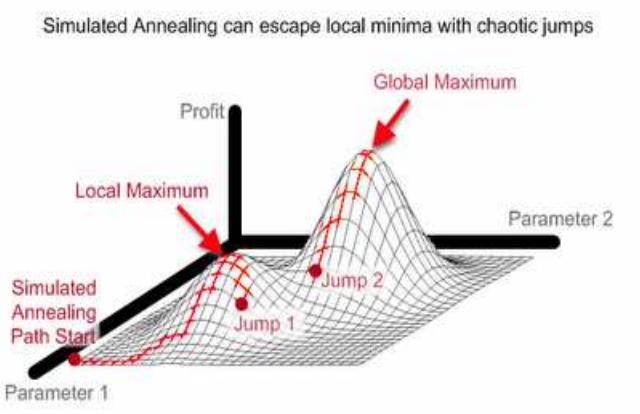

Figure 1. How to "climb mountain" for SA

Hill Climbing and Simulated Annealing

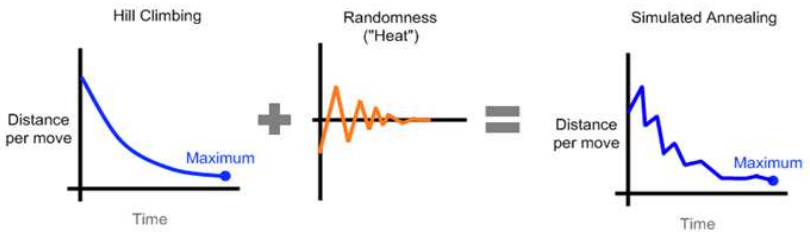

Figure 2. Hill Climbing and Simulated Annealing

Metropolis criterion

Change from E_0 to E with probability:

$$\min\left\{1, \exp\left(-\frac{E - E_0}{T}\right)\right\} \tag{3}$$

Given sufficient time, leads to equilibrium state.

Probability of state with energy k is

$$P(E = k) \propto \exp\left(-k/T\right)$$

Starting Temperature

- Must be hot enough to allow moves to almost every neighborhood state
- Must not be so hot that we conduct a random search for a long period of time
- Problem is finding a suitable starting temperature

At present, there is **no known method** for finding a suitable starting temperature for a **whole range of problems**.

However, Rayward-Smith[4] , Dowsland[1] et al, have a ideal:

First cool it rapidly to a certain percent from higher tem. , then slow down.

SA Algorithm

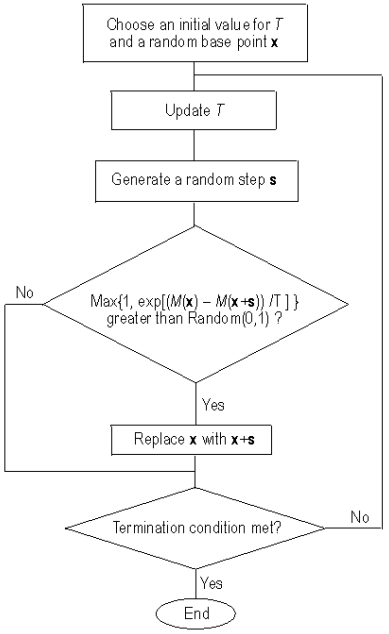

Figure 3. Flow chart of SA

SA Algorithm

I. Select starting temperature and initial parameter values

II. Randomly select a new point in the neighborhood of the original

III. Compare the two points using the Metropolis criterion

IV. Repeat steps 2 and 3 until system reaches equilibrium state...

V. Decrease temperature and repeat the above steps, stop when system reaches frozen state

SA Advantages/Disadvantages

- Advantages
  i. Guaranteed to find optimum
  ii. Avoids being trapped at local minimums

- Disadvantages
  i. Not faster than many contemporaries

References

Bibliography

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[3] Rosenbluth M.N., Teller A.H., Teller E Metropolis N., Rosenbluth A.W. Equation of state calculation by fast computing machines. *E.J. of Chem. Phys.*, 21:1087–1091, 1953.

[4] Reeves C.R., Smith G.D. Rayward-Smith V.J., Osman I.H. Smodern heuristic search methods. *John Wiley & Sons*, , 1996.