Numerical Optimization

Joachim Vandekerckhove

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- **Machine Learning:** Train a model to predict outcomes based on input features by minimizing a loss function.
- **Procedure Optimization:** Find the conditions where a certain procedure works best.

Numerical optimization in cognitive modeling

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- To-be-optimized function is called target or objective function

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4. Repeat until good enough

Numerical optimization in cognitive modeling

Algorithm: Abstract Numerical Minimization

Input : objective function $\ell(\theta)$

Output: the learned parameters θ

1. Initial guess parameters θ
2. **while** $\ell(\theta)$ is too high **do**
   Propose new parameters: $\theta \leftarrow \theta + \text{update}$;
3. **return** θ;

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- Other optimization methods include genetic algorithms, simulated annealing, particle swarm optimization, and the Nelder-Mead simplex

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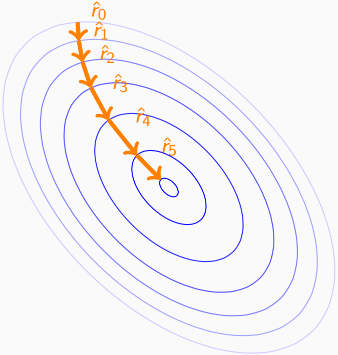

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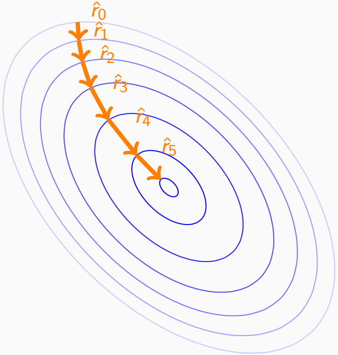

  - Some nice visualizations: https://www.benfrederickson.com/numerical-optimization/

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- The process is governed by a temperature setting that determines the probability of accepting a step in the wrong direction.
- A hot algorithm will move randomly, with little regard for the objective function value. A cold algorithm performs steepest ascent.
- A slow cooling schedule allows the algorithm to explore many possible peaks before climbing to the top.

Simulated Annealing

Algorithm 2: Simulated Annealing Algorithm

Input: Initial guess s, initial temperature T; objective $\ell(\theta)$

Output: Best parameter set found during search

while stopping condition not met **do**

  Generate new guess s' by random perturbation to s;

  Calculate loss difference $\Delta\ell = \ell(s') - \ell(s)$;

  if $\Delta E < 0$ **then**

    Accept s' as the new current state s;

  else

    Accept s' with probability $\exp(-\Delta\ell/T)$;

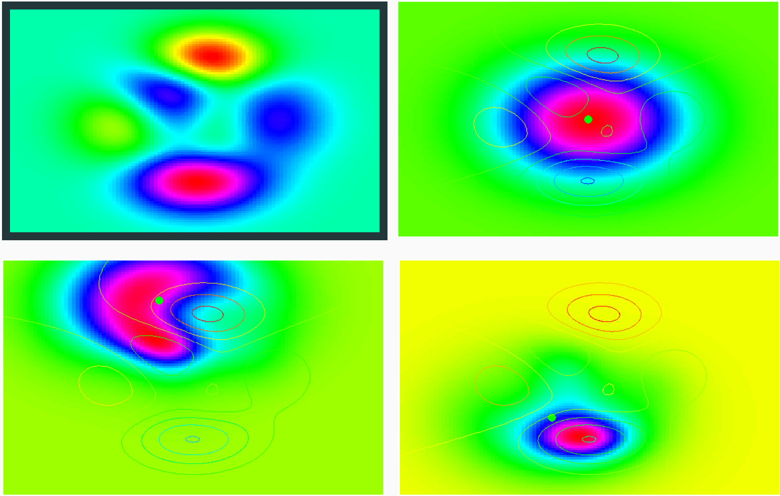
  end

  Decrease temperature T;

end

return Best state found during search

Simulated Annealing



Constrained vs. Unconstrained Optimization

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- In an unconstrained optimization problem, the goal is to minimize (or maximize) a function subject to no constraints
- In a constrained optimization problem, the goal is to minimize (or maximize) a function subject to one or more constraints
- Constrained optimization often requires the use of specialized optimization algorithms and techniques to find the global minimum (or maximum)

Constrained vs. Unconstrained Optimization

Constraints can be that some linear transformation A of the parameters must be less than some constant b, and/or that some linear transformation A_{eq} of the parameters must be equal to some constant b_{eq}, and/or that they must fall in bounds (l_b, u_b), and/or that some are integers.

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f^\top x \\ \text{subject to} \quad & \left\{ \begin{array}{c} Ax \le b \text{ (MATLAB)} \\ Ax \ge b \text{ (python)} \\ A_{eq}x = b_{eq} \\ l_b \le x \le u_b \\ x(\texttt{intflag}) \text{ are integers} \end{array} \right\} \end{aligned}$$

Unconstrained Example: Production Environment

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- The cost of production is given by:

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- What are the optimal settings to run the production process?

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- What is the best x?

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$$(\max_x) \quad f(x) \quad = \quad \binom{5}{4} \theta_H^5 (1-\theta_H)^1 \times \binom{5}{2} \theta_F^2 (1-\theta_F)^3$$

$$\text{with} \begin{cases} \theta_H & = & 1 - \Phi\left(-\frac{1}{2}d' + c\right) \\ \theta_F & = & 1 - \Phi\left(\frac{1}{2}d' + c\right) \end{cases}$$

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\Rightarrow (\min_x) \quad f(x) &= -\log\left[\theta_H^5 (1 - \theta_H)^1 \times \theta_F^2 (1 - \theta_F)^3\right] \\
&= -5 \log(\theta_H) - \log(1 - \theta_H) \\
&\quad - 2 \log(\theta_F) - 3 \log(1 - \theta_F)
\end{aligned}
$$

MATLAB

Unconstrained Optimization using `fminsearch`

$$\min_{x} \quad f(x) = e^{(x_1-2)^2+(x_2-0.5)^2}$$

- Set up the problem as an anonymous function:

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% Define the objective function
fcn = @(x) exp( (x(1)-2).^2 + (x(2)-.5).^2);
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- The solution is $x_1 = 2$ and $x_2 = 0.5$.

Unconstrained Optimization using `fminunc`

```
fcn = @(x) exp( (x(1)-2).^2 + (x(2)-.5).^2);
x0 = [0.5, 1.5];
options = optimoptions('fminunc', 'Display', 'iter', ...
                       'Algorithm', 'quasi-newton', ...
                       'MaxIterations', 1000);
[x, fval, exitflag, output] = fminunc(fcn, x0, options);
```

- `Display=iter` shows optimization progress at each iteration

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- `Display=iter` shows optimization progress at each iteration
- `Algorithm` specifies the optimization algorithm to use
- `MaxIterations` sets the maximum number of iterations
- Output variables `x`, `fval`, `exitflag`, and `output` contain the optimization results and information

fminunc vs. fmincon

Using fminunc:

```
fcn = @(x)sum((x-[5, -7, 3, 0, -11]).^2);
x0 = 0.5;
[x, fval, exitflag, output] = fminunc(fcn, x0);
```

Enforce $x \geq 0$ with fmincon:

```
fcn = @(x)sum((x-[5, -7, 3, 0, -11]).^2);
x0 = 0.5;
[x, fval, exitflag, output] = fmincon(fcn, x0, -1, 0);
```

Note that $A = -1$ and $b = 0$, so we enforce that $-x \leq 0$

MATLAB Optimization Toolbox

MATLAB has a lot of numerical optimization features.

As of September 2022, the MATLAB Optimization Toolbox User's Guide is 1,584 pages long. It is an excellent review of modern numerical optimization methods.

Python

Unconstrained Optimization using `scipy.optimize.minimize`

$$\min_x \quad f(x) = e^{(x_1-2)^2+(x_2-0.5)^2}$$

```
import numpy as np
import scipy.optimize as optim

# Define the objective function
def fcn(x):
    return np.exp((x[0]-2)**2 + (x[1]-0.5)**2)

# Set the initial point and solve the optimization problem
start = [0, 0]
x = optim.minimize(fcn, start, method='Nelder-Mead')

# The solution is x1=2 and x2=0.5
print(f"The solution is x1={x.x[0]} and x2={x.x[1]}")
```

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# Set the initial point and solve the optimization problem
x0 = [0.5, 1.5]
options = {'disp': True, 'maxiter': 1000}
x = optim.minimize(fcn, x0, method='BFGS', options=options)
```

- `'disp'`:`True` shows optimization progress at each iteration

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- `'disp':True` shows optimization progress at each iteration
- `'maxiter'` sets the maximum number of iterations
- `method='BFGS'` selects a Quasi-Newton optimization algorithm

Unconstrained vs. constrained

```
import numpy as np
import scipy.optimize as optim

# Define the objective function
def fcn(x):
    return np.sum((x - [5, -7, 3, 0, -11])**2)

# Set the initial point
x0 = 0.5
```

Unconstrained:

```
x = optim.minimize(fcn, x0)
```

Enforce $x \geq 0$ with `LinearConstraint`:

```
x = minimize(fcn, x0,
    constraints=optim.LinearConstraint(1, 0))
```

Note that $A = 1$ and $b = 0$, so we enforce that $x \geq 0$