Modern Optimization Techniques

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Newton's Method

Outline

1. Review
2. The Newton's Method

Outline

Unconstrained Optimization Problems

An **unconstrained optimization problem** has the form:

$$\text{minimize} \quad f_0(\mathbf{x})$$

Where:

- $f_0 : \mathbb{R}^n \to \mathbb{R}$ is convex, twice differentiable
- An optimal $\mathbf{x}^*$ exists and $f(\mathbf{x}^*)$ is attained and finite

Descent Methods

The next point is generated using

- A step size μ
- A direction $\Delta \mathbf{x}$ such that

$$f_0(\mathbf{x}^t + \mu \Delta \mathbf{x}^{t-1}) < f_0(\mathbf{x}^{t-1})$$

procedure DescentMethod
  input: f_0
  Get initial point $\mathbf{x}$
  repeat
    Get Update Direction $\Delta \mathbf{x}$
    Get Step Size μ
    $\mathbf{x}^{t+1} \leftarrow \mathbf{x}^t + \mu \Delta \mathbf{x}^t$
  until convergence
  return $\mathbf{x}$, $f_0(\mathbf{x})$
end procedure

Methods seen so far

- Gradient Descent:

$$\Delta \mathbf{x} = -\nabla f_0(\mathbf{x})$$

- Stochastic Gradient Descent:
  - If the function is if the form $f_0(\mathbf{x}) = \sum_{i=1}^{m} g(\mathbf{x}, i)$:
  -

$$\Delta_i \mathbf{x} = -\nabla g(\mathbf{x}, i)$$

Outline

An idea using second order approximations

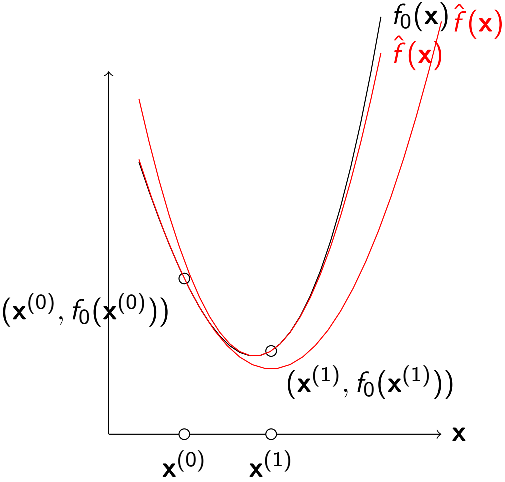
Be $f_0 : \mathbb{R}^n \to \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}$:

$$\text{minimize} \quad f_0(\mathbf{x})$$

- Start with an initial solution $\mathbf{x}^{(t)}$
- Compute $\hat{f}$, a quadratic approximation of f_0 around $\mathbf{x}^{(t)}$
- Find $\mathbf{x}^{t+1} = \arg\min \hat{f}(\mathbf{x})$
- $t \leftarrow t + 1$
- Repeat until convergence

An idea using second order approximations

$$f_0(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-3)^2 + \frac{1}{10}\mathbf{x}^3$$



Taylor Approximation

Be $f : \mathbb{R}^n \to \mathbb{R}$ an infinitely differentiable function at some point $\mathbf{a} \in \mathbb{R}^n$

$f(\mathbf{x})$ can be approximated by the Taylor expansion of f, which is given by:

$$f(\mathbf{a}) + \frac{\nabla f(\mathbf{a})}{1!}(\mathbf{x}-\mathbf{a}) + \frac{\nabla^2 f(\mathbf{a})}{2!}(\mathbf{x}-\mathbf{a})^2 + \frac{\nabla^3 f(\mathbf{a})}{3!}(\mathbf{x}-\mathbf{a})^3 + \cdots$$
$$= \sum_{i=0}^{\infty} \frac{\nabla^i f(\mathbf{a})}{i!}(\mathbf{x}-\mathbf{a})^i$$

It can be shown that for a k large enough

$$f(\mathbf{x}) = \sum_{i=0}^{k} \frac{\nabla^i f(\mathbf{a})}{i!}(\mathbf{x}-\mathbf{a})^i$$

Second Order Approximation

Let us take the second order approximation of a twice differentiable function $f_0 : \mathbb{R}^n \to \mathbb{R}$ at a point $\mathbf{x}$:

$$\hat{f}(\mathbf{t}) = f_0(\mathbf{x}) + \nabla f_0(\mathbf{x})^T(\mathbf{t} - \mathbf{x}) + \frac{1}{2}(\mathbf{t} - \mathbf{x})^T \nabla^2 f_0(\mathbf{x})(\mathbf{t} - \mathbf{x})$$

We want to find the point $\mathbf{t} = \mathbf{x}^{(t+1)} = \arg\min \hat{f}$:

$$\begin{aligned}
\nabla_{\mathbf{t}} \hat{f}(\mathbf{t}) = \nabla f_0(\mathbf{x}) + \nabla^2 f_0(\mathbf{x})(\mathbf{t} - \mathbf{x}) &\overset{!}{=} 0 \\
\nabla f_0(\mathbf{x}) + \nabla^2 f_0(\mathbf{x})(\mathbf{t} - \mathbf{x}) &= 0 \\
\nabla^2 f_0(\mathbf{x})(\mathbf{t} - \mathbf{x}) &= -\nabla f_0(\mathbf{x}) \\
\mathbf{t} - \mathbf{x} &= -\nabla^2 f_0(\mathbf{x})^{-1} \nabla f_0(\mathbf{x}) \\
\mathbf{t} &= \mathbf{x} - \nabla^2 f_0(\mathbf{x})^{-1} \nabla f_0(\mathbf{x})
\end{aligned}$$

Newton's Step

- Be $f_0 : \mathbb{R}^n \to \mathbb{R}$ a twice differentiable convex function
- Newton's step uses the inverse of the Hessian matrix $\nabla^2 f_0(\mathbf{x})^{-1}$ and the gradient $\nabla f_0(\mathbf{x})$

$$\Delta^{\text{Newton}}\mathbf{x} = -\nabla^2 f_0(\mathbf{x})^{-1} \nabla f_0(\mathbf{x})$$

Newton Decrement

We have a measure of the proximity of $\mathbf{x}$ to the optimal solution $\mathbf{x}^*$:

$$\lambda(\mathbf{x}) = \left(\nabla f_0(\mathbf{x})^T \nabla^2 f_0(\mathbf{x})^{-1} \nabla f_0(\mathbf{x})\right)^{\frac{1}{2}}$$

- It provides a useful estimate of $f_0(\mathbf{x}) - f_0(\mathbf{x}^*)$ using the quadratic approximation $\hat{f}$:

$$f_0(\mathbf{x}) - \inf_{\alpha} \hat{f}(\alpha) = \frac{1}{2}\lambda(\mathbf{x})^2$$

- it is affine invariant (insensitive to the choice of coordinates)

Newton's method

```
procedure NEWTONS METHOD
input: f_0, tolerance ε > 0
    Get initial point x
    repeat
        Δx ← −∇²f_0(x)^{-1} ∇f_0(x)
        λ² ← ∇f_0(x)^T ∇²f_0(x)^{-1} ∇f_0(x)
        if λ²/2 ≤ ε then
            Quit
        end if
        Get Step Size μ
        x ← x + μΔx
    until convergence
    return x, f_0(x)
end procedure
```

Affine Invariance

We want to minimize $f_0(\mathbf{x})$.

Be T a positive-semidefinite matrix such that: $T\alpha = \mathbf{x}$

We can minimize $\tilde{f}(\alpha) = f_0(T\alpha) = f_0(\mathbf{x})$

The gradient of $\tilde{f}$ is:

$$\nabla \tilde{f}(\alpha) = T^\top \nabla f_0(T\alpha)$$

This means that the gradient method isn't affine invariant!

Considerations

- Works extremely well for a lot of problems
- f_0 must be twice differentiable
- The Hessian has n^2 elements.
- Compute and store the Hessian might hinder it's scalability for high dimensional problems
- Inverting the Hessian might be in some cases impractical

Newton's method - Example

For $\mathbf{x} \in \mathbb{R}$

$$\min_{\mathbf{x}} \quad (2\mathbf{x} - 4)^4$$

Algorithm:

- Let us use a fixed step size $\mu = 1$
- Initialize $\mathbf{x}^{(0)}$
- Repeat until convergence:
  - $\mathbf{x}^{(t)} \leftarrow -\frac{\nabla f_0(\mathbf{x}^{(t-1)})}{\nabla^2 f_0(\mathbf{x}(t-1))}$

Newton's method - Example

For $\mathbf{x} \in \mathbb{R}$

$$\min_{\mathbf{x}} \quad (2\mathbf{x} - 4)^4$$

Algorithm:

- $\nabla f_0(\mathbf{x}) = 8(2\mathbf{x} - 4)^3$
- $\nabla^2 f_0(\mathbf{x}) = 48(2\mathbf{x} - 4)^2$
- Step: $\Delta\mathbf{x} = -\nabla^2 f_0(\mathbf{x})^{-1} \nabla f_0(\mathbf{x})$
- $\Delta\mathbf{x} = -\frac{1}{6}(2\mathbf{x} - 4)$

Newton's method - Example

We Start at $\mathbf{x}^0 = 2.5$

- $\mathbf{x}^1 \leftarrow 2.5 - \frac{1}{6}(2 \cdot 2.5 - 4) = 2.3333$
- $\mathbf{x}^2 \leftarrow 2.33333 - \frac{1}{6}(2 \cdot 2.3333 - 4) = 2.22222$
- $\mathbf{x}^3 \leftarrow 2.22222 - \frac{1}{6}(2 \cdot 2.22222 - 4) = 2.148148$
- $\mathbf{x}^4 \leftarrow 2.148148 - \frac{1}{6}(2 \cdot 2.148148 - 4) = 2.098765$
- $\mathbf{x}^5 \leftarrow 2.098765 - \frac{1}{6}(2 \cdot 2.098765 - 4) = 2.065844$
- $\mathbf{x}^6 \leftarrow 2.065844 - \frac{1}{6}(2 \cdot 2.065844 - 4) = 2.043896$
- ...
- $\mathbf{x}^{20} \leftarrow 2.000226 - \frac{1}{6}(2 \cdot 2.0000134 - 4) = 2.00015$

Practical Example: Household Location

Suppose we have the following data about different households:

- Number of workers in the household (a_1)
- Household composition (a_2)
- Weekly household spending (a_3)
- Gross normal weekly household income (a_4)
- **Region** (y): North $y = 1$ or south $y = 0$

We want to creat a model of the location of the household

Practical Example: Household Spending

If we have data about m households, we can represent it as:

$$A_{m,n} = \begin{pmatrix} 1 & a_{1,2} & \dots & a_{1,n} \\ 1 & a_{2,2} & \dots & a_{2,n} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & a_{m,2} & \dots & a_{m,n} \end{pmatrix} \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

We can model the household location is a linear combination of the household features with parameters $\mathbf{x}$:

$$\hat{y}_i = \sigma(\mathbf{x}^T \mathbf{a_i}) = \sigma(\mathbf{x}_0 1 + \mathbf{x}_1 a_{i,1} + \mathbf{x}_2 a_{i,2} + \mathbf{x}_3 a_{i,3} + \mathbf{x}_4 a_{i,4})$$

where: $\sigma(x) = \frac{1}{1+e^{-x}}$

Example II - The Logistic Regression

The logistic regression learning problem is

$$\text{minimize} \quad \sum_{i=1}^{m} y_i \log \sigma(\mathbf{x}^T \mathbf{a_i}) + (1 - y_i) \log(1 - \sigma(\mathbf{x}^T \mathbf{a_i}))$$

$$A_{m,n} = \begin{pmatrix} 1 & a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} \\ 1 & a_{2,1} & a_{2,2} & a_{2,3} & a_{2,4} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & a_{m,1} & a_{m,2} & a_{m,3} & a_{m,4} \end{pmatrix} \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

The Logistic Regression

First we need to compute the gradient of our objective function:

$$\text{minimize} \quad \sum_{i=1}^{m} y_i \log \sigma(\mathbf{x}^T \mathbf{a_i}) + (1 - y_i) \log(1 - \sigma(\mathbf{x}^T \mathbf{a_i}))$$

$$\begin{aligned}
\frac{\partial f_0}{\partial \mathbf{x}_k} &= \sum_{i=1}^{m} y_i \frac{1}{\sigma(\mathbf{x}^T \mathbf{a_i})} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(1 - \sigma(\mathbf{x}^T \mathbf{a_i})\right) a_{ik} \\
&\quad - (1 - y_i) \frac{1}{1 - \sigma(\mathbf{x}^T \mathbf{a_i})} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(1 - \sigma(\mathbf{x}^T \mathbf{a_i})\right) a_{ik} \\
&= \sum_{i=1}^{m} y_i a_{ik} \left(1 - \sigma(\mathbf{x}^T \mathbf{a_i})\right) - (1 - y_i) a_{ik} \sigma(\mathbf{x}^T \mathbf{a_i}) \\
&= \sum_{i=1}^{m} a_{ik} \left(y_i - \sigma(\mathbf{x}^T \mathbf{a_i})\right)
\end{aligned}$$

The Logistic Regression

$$\frac{\partial f_0}{\partial \mathbf{x}_k} = \sum_{i=1}^{m} a_{ik} \left(y_i - \sigma(\mathbf{x}^T \mathbf{a_i}) \right)$$

Now we need to compute the Hessian matrix:

$$\begin{aligned}\frac{\partial^2 f_0}{\partial \mathbf{x}_k \partial \mathbf{x}_j} &= \sum_{i=1}^{m} -a_{ik} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(1 - \sigma(\mathbf{x}^T \mathbf{a_i})\right) a_{ij} \\ &= \sum_{i=1}^{m} a_{ik} a_{ij} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(\sigma(\mathbf{x}^T \mathbf{a_i}) - 1\right)\end{aligned}$$

The Hessian H is an $n \times n$ matrix such that:

$$H_{k,j} = \sum_{i=1}^{m} a_{ik} a_{ij} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(\sigma(\mathbf{x}^T \mathbf{a_i}) - 1\right)$$

The Logistic Regression

So we have our gradient $\nabla f_0 \in \mathbb{R}^n$ such that

$$\nabla_{\mathbf{x}_k} f_0 = \sum_{i=1}^{m} a_{ik} \left(y_i - \sigma(\mathbf{x}^T \mathbf{a_i}) \right)$$

And the Hessian $H \in \mathbb{R}^{n \times n}$:

$$H_{k,j} = \sum_{i=1}^{m} a_{ik} a_{ij} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(\sigma(\mathbf{x}^T \mathbf{a_i}) - 1 \right)$$

the newton update rule is:

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \mu H^{-1} \nabla f_0$$

Newton's Method for Logistic Regression - Considerations

The newton update rule is:

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \mu H^{-1} \nabla f_0$$

Biggest problem:

How to efficiently compute H^{-1} for:

$$H_{k,j} = \sum_{i=1}^{m} a_{ik} a_{ij} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(\sigma(\mathbf{x}^T \mathbf{a_i}) - 1 \right)$$

Considerations:

- H is symmetric: $H_{k,j} = H_{j,k}$