Modern Optimization Techniques

2. Unconstrained Optimization / 2.3. Newton's Method

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Outline

Outline

1. Newton's Method
2. Convergence
3. Example: Logistic Regression

An idea using second order approximations

Be $f : X \to \mathbb{R}, X \subseteq \mathbb{R}^N$ open and f convex:

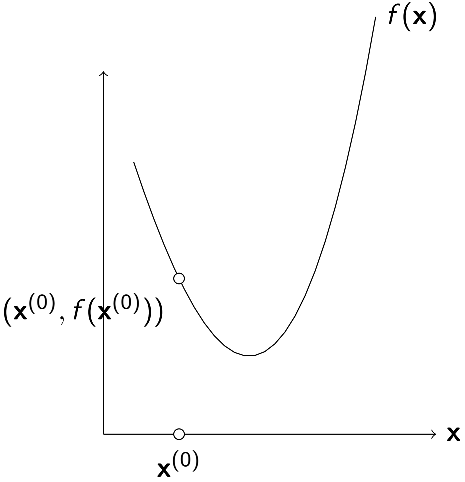
$$\arg\min_{x \in X} \quad f(\mathbf{x})$$

- Let $\mathbf{x}^{(k)}$ the last iterate
- Compute a quadratic approximation $\hat{f}$ of f around $\mathbf{x}^{(k)}$
- Find the minimum of the quadratic approximation $\hat{f}$ and take it as next iterate:

$$\mathbf{x}^{(k+1)} := \arg\min_{x \in X} \hat{f}(\mathbf{x})$$

An idea using second order approximations

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



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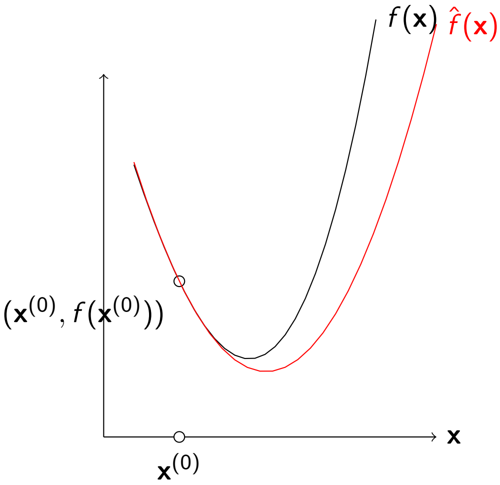

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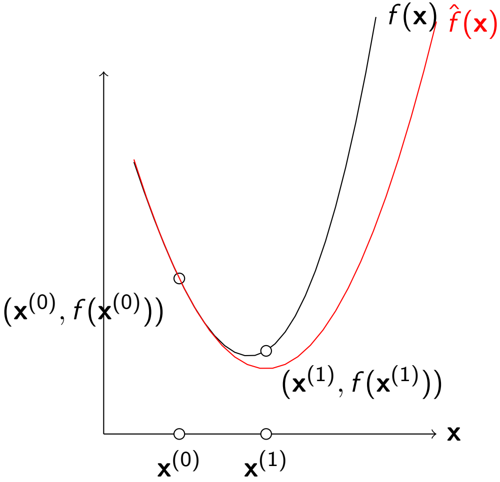

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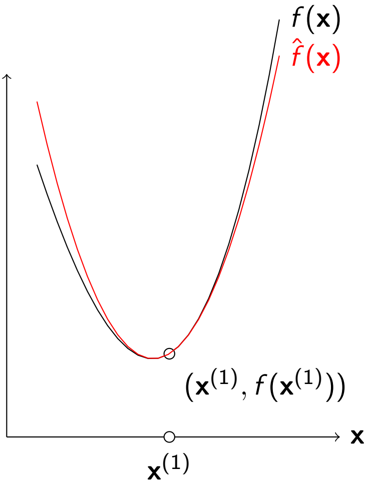

Taylor Approximation

Be $f : X \to \mathbb{R}, X \subseteq \mathbb{R}^N$ an infinitely differentiable function, $\mathbf{a} \in X$ any point.

f can be represented by its **Taylor expansion**:

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

For x close enough to a and K large enough,
f can be approximated by its **truncated Taylor expansion**:

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

Note: For $N > 1$, $\nabla^k f(x)$ is a tensor of order k and $\nabla^k f(x)(x-a)^k$ a tensor product.

Second Order Approximation

Let us take the second order approximation of a twice differentiable function $f : X \to \mathbb{R}, X \subseteq \mathbb{R}^N$ at a point $\mathbf{x}$:

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

We want to find the point $x^{\text{next}} := \arg\min_y \hat{f}(y)$:

$$\nabla_{\mathbf{y}} \hat{f}(\mathbf{y}) = \nabla f(\mathbf{x}) + \nabla^2 f(\mathbf{x})(\mathbf{y}-\mathbf{x}) \overset{!}{=} 0$$

$$\rightsquigarrow \quad \mathbf{y} = \mathbf{x} - \nabla^2 f(\mathbf{x})^{-1} \nabla f(\mathbf{x})$$

Newton's Step

- Newton's method is a descent method

- It uses the descent direction

$$\Delta \mathbf{x} := -\nabla^2 f(\mathbf{x})^{-1} \nabla f(\mathbf{x})$$

  called **Newton step**.
  - the negative gradient
  - twisted by the local curvature (Hessian)

- Newton's step is affine invariant,
  while the gradient step is not.

Newton's Step / Proof

(i) Show that the Gradient step is not affine invariant.
for $g(y) := f(Ay)$ with a pos.def. matrix A

$$\nabla_y g(y) = A^T \nabla_x f(Ay) \stackrel{?}{=} A^{-1} \nabla_x f(x), \quad \text{for } x := Ay$$

No, as in general $A^T \neq A^{-1}$.

(ii) Show that Newton's step is affine invariant.

$$\begin{aligned}
\nabla_y^2 g(y) &= A^T \nabla_x^2 f(Ay) A \\
\Delta y &= (\nabla_y^2 g(y))^{-1} \nabla_y g(y) \\
&= A^{-1} \nabla_x^2 f(Ay)^{-1} (A^T)^{-1} A^T \nabla_x f(Ay) \\
&= A^{-1} \nabla_x^2 f(Ay)^{-1} \nabla_x f(Ay) \\
&= A^{-1} \nabla_x^2 f(x)^{-1} \nabla_x f(x), \quad \text{for } x := Ay
\end{aligned}$$

Newton's Stepsize

- For quadratic objective functions f:
  - Newton's method will find the optimum in a single step
    - with stepsize 1

    (**pure Newton**)
- For general objective functions:
  - a possibly smaller stepsize has to be used
    (**damped Newton**)
  - any stepsize controller is applicable

Newton Decrement

$$\lambda(x) := (\nabla f(x)^T \nabla^2 f(x)^{-1} \nabla f(x))^{\frac{1}{2}}$$

is called **newton decrement**.

Basic properties:

(i)

$$\lambda(x) = (\Delta x^T \nabla^2 f(x) \Delta x)^{\frac{1}{2}}$$

(ii)

$$\lambda(x)^2 = -\nabla f(x)^T \Delta x$$

(iii)

$$f(x) - \inf_y \hat{f}(y) = f(x) - \hat{f}(x + \Delta x) = \frac{1}{2}\lambda(x)^2$$

(iv) The Newton decrement is affine invariant.

Newton Decrement / Proofs

i), (ii) insert the definition of $\Delta x = -\nabla^2 f(x)^{-1} \nabla f(x)$

nd (iii)

$$f(x) - \hat{f}(x + \Delta x) = f(x) - f(x) \underbrace{-\nabla f(x)^T \Delta x}_{\stackrel{ii}{=} \lambda(x)^2} - \frac{1}{2} \underbrace{\Delta x^T \nabla^2 f(x) \Delta x}_{\stackrel{i}{=} \lambda(x)^2}$$

nd (iv) for $g(y) := f(Ay)$ with a pos.def. matrix A

$$\nabla_y g(y) = A^T \nabla_x f(Ay), \quad \nabla_y^2 g(y) = A^T \nabla_x^2 f(Ay) A$$
$$\lambda_g(y) = \nabla_x f(Ay)^T A A^{-1} \nabla_x^2 f(Ay)^{-1} (A^T)^{-1} A^T \nabla_x f(Ay)^T$$
$$= \nabla_x f(Ay)^T \nabla_x^2 f(Ay)^{-1} \nabla_x f(Ay)^T$$
$$= \lambda_f(x) \text{ at } x := Ay$$

Newton's Method

min-newton$(f, \nabla f, \nabla^2 f, x^{(0)}, \mu, \epsilon, K)$:
  for $k := 1, \ldots, K$:
    $\Delta x^{(k-1)} := -\nabla^2 f(x^{(k-1)})^{-1} \nabla f(x^{(k-1)})$
    if $-\nabla f(x^{(k-1)})^T \Delta x^{(k-1)} < \epsilon$:
      return $x^{(k-1)}$
    $\mu^{(k-1)} := \mu(f, x^{(k-1)}, \Delta x^{(k-1)})$
    $x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)}$
  return "not converged"

where

- f objective function
- ∇f, $\nabla^2 f$ gradient and Hessian of objective function f
- $x^{(0)}$ starting value
- μ step length controller
- ϵ convergence threshold for Newton's decrement
- K maximal number of iterations

Considerations

- Works extremely well for a lot of problems
- requires f to be twice differentiable
- Computing, storing and inverting the Hessian limits scalability for high dimensional problems
  - as the Hessian has N^2 elements.

Newton's method - Example

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

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

Algorithm:

- $\nabla f(\mathbf{x}) = 8\,(2\mathbf{x} - 4)^3$
- $\nabla^2 f(\mathbf{x}) = 48\,(2\mathbf{x} - 4)^2$
- Step:

$$\begin{aligned}\Delta\mathbf{x} &= \nabla^2 f(\mathbf{x})^{-1} \nabla f(\mathbf{x}) \\ &= -\frac{1}{6}(2\mathbf{x} - 4)\end{aligned}$$

- Update:

$$\begin{aligned}x^{(k+1)} &= x^{(k)} + \mu^{(k)} \Delta x^{(k)} \\ &= x^{(k)} - \frac{1}{6}(2x^{(k)} - 4)\end{aligned}$$

Newton's method - Example

$$x^{(0)} := 10$$

$$x^{(1)} = 10.0 - \frac{1}{6}(2 \cdot 10.0 - 4) = 7.33333$$

$$x^{(2)} = 7.33333 - \frac{1}{6}(2 \cdot 7.33333 - 4) = 5.55556$$

$$x^{(3)} = 5.55556 - \frac{1}{6}(2 \cdot 5.55556 - 4) = 4.37037$$

$$x^{(4)} = 4.37037 - \frac{1}{6}(2 \cdot 4.37037 - 4) = 3.58025$$

$$x^{(5)} = 3.58025 - \frac{1}{6}(2 \cdot 3.58025 - 4) = 3.0535$$

$$x^{(6)} = 3.0535 - \frac{1}{6}(2 \cdot 3.0535 - 4) = 2.70233$$

$$x^{(7)} = 2.70233 - \frac{1}{6}(2 \cdot 2.70233 - 4) = 2.46822$$

$$x^{(8)} = 2.46822 - \frac{1}{6}(2 \cdot 2.46822 - 4) = 2.31215$$

Outline

Newton Decrement / Strongly Convex Functions

If f is strongly convex ($\nabla^2 f(x) \succeq mI, m \in \mathbb{R}^+$), then

(i)

$$m||\Delta x||_2^2 \leq \lambda(x)^2 \leq M||\Delta x||_2^2$$

(ii)

$$\frac{1}{M}||\nabla f(x)||_2^2 \leq \lambda(x)^2 \leq \frac{1}{m}||\nabla f(x)||_2^2$$

where $\nabla^2 f(x) \preceq MI, M \in \mathbb{R}^+$.

Newton Decrement / Strongly Convex Functions / Proofs

ad (i)

$$\lambda(x)^2 = \Delta x^T \nabla^2 f(x) \Delta x \geq m ||\Delta x||_2^2$$
$$\lambda(x)^2 = \Delta x^T \nabla^2 f(x) \Delta x \leq M ||\Delta x||_2^2$$

ad (ii) The inverse of $\nabla^2 f(x)$ has inverse eigenvalues, thus

$$\nabla^2 f(x)^{-1} \preceq \frac{1}{m} I$$
$$\nabla^2 f(x)^{-1} \succeq \frac{1}{M} I$$

Then proceed as (i).

Convergence / Assumptions

Until the end of this section, assume

I. f is strongly convex (m, M),

II. $\nabla^2 f(x)$ is Lipschitz-continuous:
$||\nabla^2 f(y) - \nabla^2 f(x)||_2 \leq L||y - x||_2, \quad L \in \mathbb{R}^+$ and

III. backtracking steplength control is used $(\alpha \leq \frac{1}{2}, \beta)$

Convergence / Damped Phase

Theorem (Convergence of Newton's Algorithm / Damped Phase)

Far away from the optimum,

(i) *backtracking may select stepsizes* $t \leq 1$ *(be damped) and*

(ii) f *is reduced by at least a constant each step.*

$$\text{for } \nabla ||f(x)||_2 \geq \eta : \; f(x^{next}) - f(x) \leq -\gamma$$
$$\text{with } \gamma := \alpha\beta \frac{m}{M^2}\eta^2$$

Convergence / Damped Phase / Proof

$$f(x + t\Delta x) \underset{\text{s.c. ii}}{\leq} f(x) + t\nabla f(x)^T \Delta x + \frac{M}{2}||\Delta x||_2^2 t^2$$

$$\underset{\text{dec. ii}}{\leq} f(x) - t\lambda(x)^2 + \frac{M}{2m} t^2 \lambda(x)^2 \tag{1}$$

$\hat{t} := m/M$ satisfies exit condition of backtracking:

$$f(x + \hat{t}\Delta x) \underset{(1)}{\leq} f(x) - \frac{m}{M}\lambda(x)^2 + \frac{m}{2M}\lambda(x)^2$$

$$= f(x) - \frac{m}{2M}\lambda(x)^2$$

$$\underset{\alpha \leq \frac{1}{2}}{\leq} f(x) - \alpha \hat{t} \lambda(x)^2$$

and thus stepsize

$$t \geq \beta \frac{m}{M} \tag{2}$$

Convergence / Damped Phase / Proof (2/2)

$$
\begin{aligned}
f(x^{\text{next}}) - f(x) &\leq -\alpha t \lambda(x)^2 \\
&\underset{(2)}{\leq} -\alpha\beta \frac{m}{M} \lambda(x)^2 \\
&\underset{\text{dec s.c. ii}}{\leq} -\alpha\beta \frac{m}{M^2} ||\nabla f(x)||_2^2 \\
&\underset{||\nabla f(x)||_2 \geq \eta}{\leq} -\alpha\beta \frac{m}{M^2} \eta^2 = -\gamma
\end{aligned}
$$

Convergence / Pure Phase

Theorem (Convergence of Newton's Algorithm / Pure Phase)

Close to the optimum,

(i) *backtracking always selects stepsize* $t = 1$ *and*

(ii) $\nabla f(x)$ *is shrunken quadratically.*

$$\textit{for } ||\nabla f(x)||_2 < \eta: \; ||\nabla f(x^{next})||_2 \leq \frac{L}{2m^2}(||\nabla f(x)||_2)^2$$

$$\textit{with } \eta \leq 3(1-2\alpha)\frac{m^2}{L}$$

(iii) *it stays close to the optimum.*

$$\textit{for } ||\nabla f(x)||_2 < \eta: \; ||\nabla f(x^{next})||_2 < \eta$$

$$\textit{with } \eta := \min\{1, 3(1-2\alpha)\}\frac{m^2}{L}$$

Convergence / Pure Phase / Proof (1/6)

(i) show backtracking accepts stepsize $t = 1$, if $\eta \leq 3(1-2\alpha)\frac{m^2}{L}$

$$||\nabla^2 f(x + t\Delta) - \nabla^2 f(x)||_2 \underset{\text{II}}{\leq} tL||\Delta x||_2$$

$$\begin{aligned} \rightsquigarrow \ |\Delta x^T(\nabla^2 f(x+t\Delta x) - \nabla^2 f(x))\Delta x| & \\ & \leq ||\nabla^2 f(x+t\Delta x) - \nabla^2 f(x)||_2 ||\Delta x||_2^2 \\ & = tL||\Delta x||_2^3 \end{aligned} \quad (1)$$

Convergence / Pure Phase / Proof (2/6)

Compute a lower bound for

$$\tilde{f}(t) := f(x + t\Delta x)$$

$$\tilde{f}'(t) = \Delta x^T \nabla f(x + t\Delta x)$$

$$\tilde{f}''(t) = \Delta x^T \nabla^2 f(x + t\Delta x)\Delta x$$

$$|\tilde{f}''(t) - \tilde{f}''(0)| \underset{(1)}{\leq} tL||\Delta x||_2^3$$

$$\tilde{f}''(t) \leq \tilde{f}''(0) + tL||\Delta x||_2^3$$

$$\underset{\text{dec i, dec s.c. i}}{\leq} \lambda(x)^2 + t\frac{L}{m^{\frac{3}{2}}}\lambda(x)^3 \qquad | \int_0^1 (\ldots)dt$$

$$\tilde{f}'(t) \leq \tilde{f}'(0) + t\lambda(x)^2 + t^2\frac{L}{2m^{\frac{3}{2}}}\lambda(x)^3$$

$$\underset{\text{dec ii}}{\leq} -\lambda(x)^2 + t\lambda(x)^2 + t^2\frac{L}{2m^{\frac{3}{2}}}\lambda(x)^3$$

Convergence / Pure Phase / Proof (3/6)

$$\tilde{f}'(t) \leq -\lambda(x)^2 + t\lambda(x)^2 + t^2 \frac{L}{2m^{\frac{3}{2}}}\lambda(x)^3 \qquad | \int_0^1 (\ldots)dt$$

$$\tilde{f}(t) \leq \tilde{f}(0) - t\lambda(x)^2 + \frac{1}{2}t^2\lambda(x)^2 + t^3 \frac{L}{6m^{\frac{3}{2}}}\lambda(x)^3 \qquad |t = 1$$

$$f(x + \Delta x) = \tilde{f}(1) \leq \tilde{f}(0) - \lambda(x)^2 + \frac{1}{2}\lambda(x)^2 + \frac{L}{6m^{\frac{3}{2}}}\lambda(x)^3$$

$$= f(x) - \lambda(x)^2(\frac{1}{2} - \frac{L}{6m^{\frac{3}{2}}}\lambda(x)) \qquad (2)$$

Convergence / Pure Phase / Proof (4/6)

$$\begin{aligned}
\lambda(x) &\underset{\text{dec s.c. ii}}{\leq} \frac{1}{m^{\frac{1}{2}}}||\nabla f(x)||_2 \\
&\underset{||\nabla f(x)||_2<\eta}{<} \frac{1}{m^{\frac{1}{2}}}\eta = \frac{1}{m^{\frac{1}{2}}}3(1-2\alpha)\frac{m^2}{L} = 3(1-2\alpha)\frac{m^{\frac{3}{2}}}{L} \qquad (3) \\
f(x+\Delta x) &\underset{(2)}{\leq} f(x) - \lambda(x)^2(\frac{1}{2} - \frac{L}{6m^{\frac{3}{2}}}\lambda(x)) \\
&\underset{(3)}{\leq} f(x) - \lambda(x)^2(\frac{1}{2} - \frac{L}{6m^{\frac{3}{2}}}3(1-2\alpha)\frac{m^{\frac{3}{2}}}{L}) \\
&= f(x) - \alpha\lambda(x)^2
\end{aligned}$$

and thus stepsize $t = 1$ fulfils the exit condition.

Convergence / Pure Phase / Proof (5/6)

(ii) show decrease in $\nabla f(x^{\text{next}})$:

$$\begin{aligned}
||\nabla f(x^{\text{next}})||_2 &\underset{t=1}{=} ||\nabla f(x + \Delta x)||_2 \\
&\underset{\text{def } \Delta x}{=} ||\nabla f(x + \Delta x) - \nabla f(x) - \nabla^2 f(x)\Delta x||_2 \\
&\underset{(*)}{=} || \int_0^1 (\nabla^2 f(x + t\Delta x) - \nabla^2 f(x))\Delta x \; dt||_2 \\
&\leq \int_0^1 ||(\nabla^2 f(x + t\Delta x) - \nabla^2 f(x))||_2 dt \; ||\Delta x||_2 \\
&\underset{\text{II}}{\leq} \int_0^1 Lt||\Delta x||_2 dt||\Delta x||_2 = \frac{1}{2} L||\Delta x||_2^2 \\
&\underset{\text{def } \Delta x}{=} \frac{1}{2} L||\nabla^2 f(x)^{-1}\nabla f(x)||_2^2 \\
&\underset{\text{dec s.c. ii}}{\leq} \frac{L}{2m^2}||\nabla f(x)||_2^2
\end{aligned}$$

where (*) $\nabla f(x + \Delta x) = \nabla^2 f(x)\Delta x + \int_0^1 \nabla^2 f(x + t\Delta x)\Delta x \; dt$

Convergence / Pure Phase / Proof (6/6)

(iii) show that Newton stays close to the optimum:

$$||\nabla f(x^{\text{next}})||_2 \underset{ii}{\leq} \frac{L}{2m^2}||\nabla f(x)||_2^2 \leq \frac{L}{2m^2}\eta^2 \underset{\text{def }\eta}{\leq} \frac{1}{2}\eta < \eta$$

Convergence

Theorem (Convergence of Newton's Algorithm)

If

(i) f *is strongly convex* (m, M)*,*

(ii) $\nabla^2 f(x)$ *is Lipschitz-continuous:*
$||\nabla^2 f(y) - \nabla^2 f(x)||_2 \leq L||y - x||_2, \quad L \in \mathbb{R}^+$ *and*

(iii) *backtracking steplength control is used* $(\alpha \leq \frac{1}{2}, \beta)$

then

$$f(x^{(k)}) - p^* \leq \frac{2m^3}{L^2} \left(\frac{1}{2}\right)^{2^{k-l+1}}, \quad k \geq l$$

$$l := \lceil \frac{f(x^{(0)}) - p^*}{\gamma} \rceil, \quad \gamma := \alpha\beta \frac{m}{M^2}\eta^2, \quad \eta := \min\{1, 3(1-2\alpha)\}\frac{m^2}{L}$$

(quadratic convergence)

Convergence / Proof

- If initially we are far away from the minimum, latest after l steps we must be close (damped phase ii) and then

$$\frac{L}{2m^2}\nabla f(x^{(l)}) \leq \frac{L}{2m^2}\eta \leq \frac{L}{2m^2}\frac{m^2}{L} \leq \frac{1}{2} \tag{1}$$

- In the pure phase $k > l$ we have (pure phase ii)

$$\frac{L}{2m^2}\nabla f(x^{(k)}) \leq (\frac{L}{2m^2}\nabla f(x^{(k-1)}))^2 \underset{\text{rec}}{\leq} (\frac{L}{2m^2}\nabla f(x^{(l)}))^{2^{k-l}} \underset{(1)}{\leq} (\frac{1}{2})^{2^{k-l}}$$

$$\nabla f(x^{(k)}) \leq \frac{2m^2}{L}(\frac{1}{2})^{2^{k-l}} \tag{2}$$

$$f(x^{(k)}) - p^* \underset{\text{s.c. i}}{\leq} \frac{1}{2m}||\nabla f(x^{(k)})||_2^2 \underset{(2)}{\leq} \frac{1}{2m}\left(\frac{2m^2}{L}(\frac{1}{2})^{2^{k-l}}\right)^2$$

$$= \frac{2m^3}{L^2}(\frac{1}{2})^{2^{k-l+1}}$$

Outline

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 - Logistic Regression

The logistic regression learning problem is

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

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

Logistic Regression

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

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

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

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

Logistic Regression

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

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

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

$$-(1 - y_i) \frac{1}{1 - \sigma(\mathbf{x}^T \mathbf{a_i})} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(1 - \sigma(\mathbf{x}^T \mathbf{a_i})\right) a_{ik}$$

Logistic Regression

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

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

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

$$-(1 - y_i) \frac{1}{1 - \sigma(\mathbf{x}^T \mathbf{a_i})} \sigma(\mathbf{x}^T \mathbf{a_i}) \left(1 - \sigma(\mathbf{x}^T \mathbf{a_i})\right) a_{ik}$$

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

Logistic Regression

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

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

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

Logistic Regression

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

Now we need to compute the Hessian matrix:

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

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

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

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

Logistic Regression

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

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

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:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mu H^{-1} \nabla f$$

Newton's Method for Logistic Regression - Considerations

The newton update rule is:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mu H^{-1} \nabla f$$

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: $H_{k,j} = H_{j,k}$

Summary

- Newton's method approximates the objective function by means of a quadratic truncated Taylor expansion around last iterate $x^{(k)}$.

$$\hat{f}(x) = f_0 + g_0^T(x - x_0) + \frac{1}{2}(x - x_0)^T H_0 (x - x_0)$$

  - requires current position $x_0 := x^{(k)}$, function value $f_0 := f(x^{(k)})$, gradient $g_0 := \nabla f(x^{(k)})$ and Hessian $H_0 := \nabla^2 f(x^{(k)})$

- Newton's method is a descent method where the descent direction called Newton step Δx is computed as solution of a linear system of equations:

$$H_0 \Delta x = -g_0$$

  - Newton step is affine invariant.

Summary (2/2)

- Newton's method works very well for many problems.
  - requires objective to be twice differentiable.
  - but often too slow for high-dimensional problems (with many variables)
    - as Hessian has size N^2 and solving for the Newton step is $O(N^3)$
- Convergence of Newton's method decomposes in two phases:
  - damped phase:
    - far away from the optimum
    - requires step length control
    - f reduced by at least a constant per step
  - pure phase:
    - close to the optimum
    - always steplength 1 can be chosen
    - f-distance to minimum shrinks double exponentially in the number of steps
      $((\frac{1}{2})^{2^k}$; quadratic convergence).

Further Readings

- Newton's method including convergence proof
  - [Boyd and Vandenberghe, 2004, ch. 9.5]

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References I

Stephen Boyd and Lieven Vandenberghe. *Convex Optimization*. Cambridge Univ Press, 2004.