CS545: Gradient Descent

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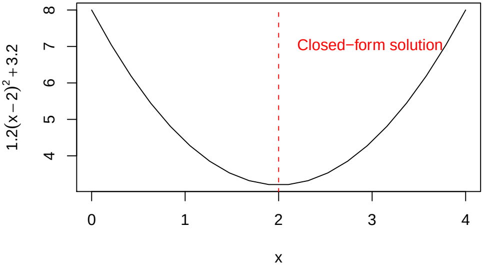
Outline

Finding Minimum of Parabola

- Find x that is minimum of $f(x) = 1.2(x-2)^2 + 3.2$ or, said another way, find $\text{argmax}_x\, f(x)$. How?
- Yep. Take derivative, set equal to zero, and try to solve for x.

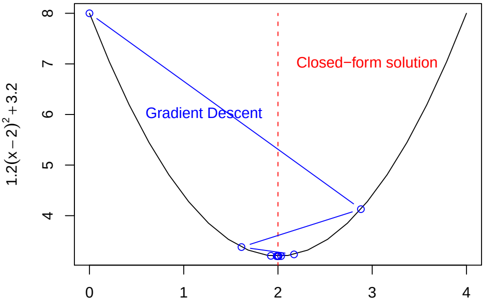
$$
\begin{aligned}
f(x) &= 1.2(x-2)^2 + 3.2 \\
\frac{df(x)}{dx} &= 1.2(2)(x-2) = 2.4(x-2) \\
\frac{df(x)}{dx} &= 0 = 2.4(x-2) \\
x &= 2
\end{aligned}
$$



Gradient Descent

- But, if $\frac{df(x)}{dx}$ is cannot be solved directly for x, what can we do?
- Start at some x value, use derivative at that value to tell us which way to move, and repeat. Gradient descent.
- ρ is factor of derivative to control how far to go

$$\frac{df(x)}{dx} = 2.4(x-2)$$
$$x(0) = 0 \text{ (for example)}$$
$$x(n) = x(n-1) - \rho\, 2.4(x-2)$$

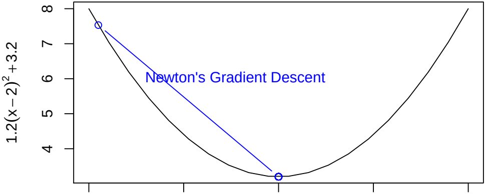


- For a parabola, can get there much faster if we also know the second derivative, which is what?

$$\frac{df(x)}{dx} = f' = 2.4(x-2)$$
$$\frac{d^2f(x)}{dx^2} = f'' = 2.4$$

- and use Newton's method (see the Wikipedia entry for "Newton's method")

$$x(n) = x(n-1) - \frac{f'}{f''}$$
$$x(n) = x(n-1) - \frac{2.4(x-2)}{2.4}$$
$$x(n) = x(n-1) - (x-2)$$



Gradient Descent

- If the function is not a parabola, what can we do? Cannot solve directly for x. Can still do gradient descent. Can we always use Newton's method?
- No. Reason 1: If x has 1000 components, the second derivative (Hessian) is a 1000×1000 matrix. May be too big.
- Reason 2: If not a parabola the second derivative information may lead you very far away. When?

Approximating the Second Derivative

- Say we have picked a direction, p, to go. Rather than compute the second derivative in that direction, we can approximate it using two first derivative values.

$$f''(x)p \approx \frac{f'(x+\alpha p) - f'(x)}{\alpha} \text{ for } 0 < \alpha << 1$$

- In practice, Moller found he had to modify this by adding λp where λ is set to a value for which the resulting approximated second derivative is well behaved.

$$f''(x)p \approx \frac{f'(x+\alpha p) - f'(x)}{\alpha} + \lambda p, \text{ for } 0 < \alpha << 1$$

- This gives us a way to scale the step size.

Picking a Good Direction

- Now, how about that direction? How do we decide that?
- Moller uses conjugate gradients. (See the wikipedia entry for "conjugate gradient")
- The conjugate gradient direction is based on the previous direction and the current gradient.

Parabola Example

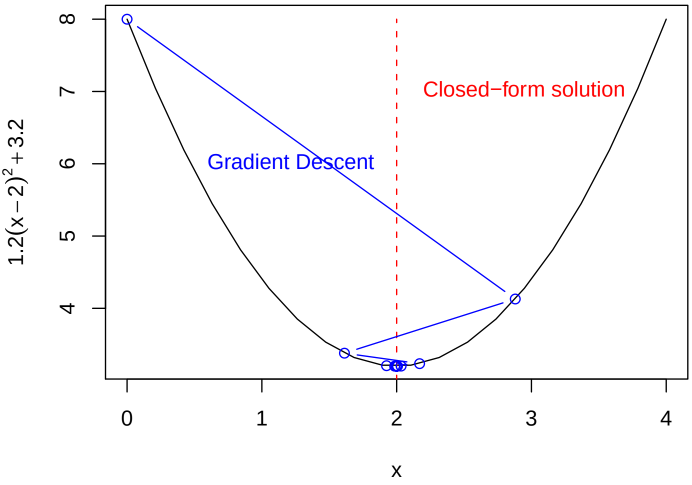
```
f <- function(x) {
  1.2 * (x-2)^2 + 3.2
}

grad <- function(x) {
  1.2 * 2 * (x-2)
}

secondGrad <- function(x) {
  2.4
}
```

Steepest Descent

```r
xs <- seq(0,4,len=20)
plot(xs, f(xs), type="l",xlab="x",ylab=expression(1.2(x-2)^2 +3.2))
### df/dx = 2.4(x-2)
### df/dx = 0 ---> 0 = 2.4x - 4.8 ---> x = 2
lines(c(2,2), c(3,8), col="red",lty=2)
text(2.1,7,"Closed-form solution",col="red",pos=4)
### gradient descent
x <- 0.1
xtrace <- x
ftrace <- f(x)
stepFactor <- 0.6 ### try larger and smaller values (0.8 and 0.01)
for (step in 1:100) {
  x <- x - stepFactor * grad(x)
  xtrace <- c(xtrace,x)
  ftrace <- c(ftrace,f(x))
}
lines(xtrace, ftrace, type="b",col="blue")
text(0.5,6,"Gradient Descent",col="blue",pos=4)
```


Closed−form solution
Gradient Descent
8
7
6
5
4
0
1
2
3
4
x
1.2(x − 2)^2 + 3.2

Steepest Descent with gradientDescents.R

```
source("gradientDescents.R")
x <- 0.1
result <- steepest(x, f, grad, stepsize=0.6, nIterations=100, xtracep=TRUE, ftracep=TRUE)
plot(xs,f(xs),type="l",xlab="x",ylab=expression(1.2(x-2)^2 +3.2))
lines(result$xtrace,result$ftrace,type="b",col="blue")
text(0.5,6,"Gradient Descent with steepest()",col="blue",pos=4)
```

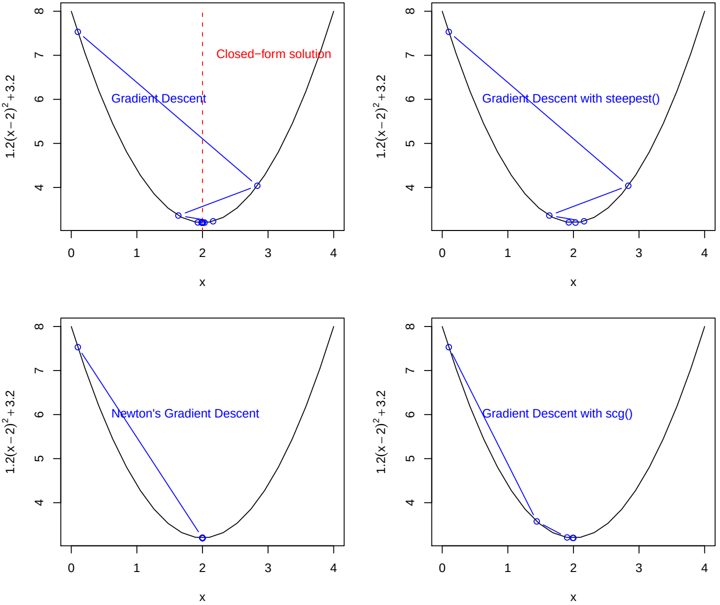
Steepest Descent scaled with Newton's Method

```r
plot(xs,f(xs),type="l",xlab="x",ylab=expression(1.2(x-2)^2 +3.2))
x <- 0.1
xtrace <- x
ftrace <- f(x)
for (step in 1:100) {
  x <- x - grad(x)/secondGrad(x)
  xtrace <- c(xtrace,x)
  ftrace <- c(ftrace,f(x))
}
lines(xtrace, ftrace,type="b",col="blue")
text(0.5,6,"Newton's Gradient Descent",col="blue",pos=4)
```

With Scaled Conjugate Gradient from gradientDescents.R

```
source("gradientDescents.R")
x <- 0.1
 result  <- scg(x, f, grad,  nIterations =100, xtracep=TRUE, ftracep=TRUE)
plot(xs,f(xs),type="l",xlab="x",ylab=expression(1.2(x-2)^2 +3.2))
 lines ( result $xtrace, result $ ftrace ,type="b",col="blue")
text (0.5,6,"Gradient  Descent with scg()", col="blue",pos=4)
```

Results



Closed−form solution
Gradient Descent
Gradient Descent with steepest()
Newton's Gradient Descent
Gradient Descent with scg()
1.2(x − 2)^2 + 3.2
x