Gov 2001 Section 3: Optimization

Konstantin Kashin [1]

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[1] Thank you to the previous TFs of Gov 2001, particularly Jen Pan and Brandon Stewart for contributing substantially to this material.

Outline

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Bernoulli Example

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The model:

1. $Y_i \sim f_{\text{bern}}(y_i|\pi_i)$.
2. $\pi_i = \pi$.
3. Y_i and Y_j are independent for all $i \neq j$.

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2. So what's the joint distribution for our data conditional on π?

$$\begin{aligned} P(\boldsymbol{y}|\pi) &= P(Y_1 = 1, Y_2 = 0, \ldots, Y_5 = 1|\pi) \\ &= P(Y_1 = 1|\pi) \cdot P(Y_2 = 0|\pi) \cdots P(Y_5 = 1|\pi) \\ &= \pi \cdot (1-\pi) \cdot (1-\pi) \cdot \pi \cdot \pi \\ &= \pi^3 (1-\pi)^2 \end{aligned}$$

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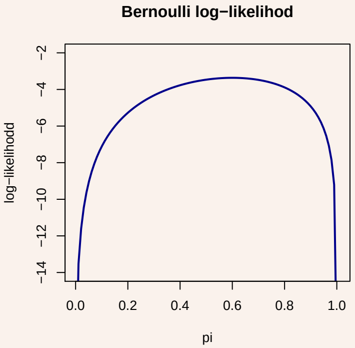
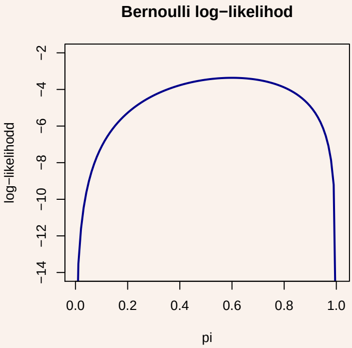
$$\begin{aligned} \ln\left[\pi^3(1-\pi)^2\right] &= \ln(\pi^3) + \ln((1-\pi)^2) \\ &= 3\ln\pi + 2\ln(1-\pi) \end{aligned}$$


Bernoulli log−likelihod
log−likelihodd
−2
−4
−6
−8
−10
−12
−14
0.0
0.2
0.4
0.6
0.8
1.0
pi



Where is the maximum, and how could we find it analytically using

$$\ln L(\pi|\boldsymbol{y}) = 3\ln\pi + 2\ln(1-\pi)?$$

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\frac{\partial \ln L(\pi|\boldsymbol{y})}{\partial \pi} &= \frac{\partial}{\partial \pi}\left[3 \ln \pi + 2 \ln(1-\pi)\right] \\
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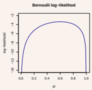
When this function is equal to zero, $\pi = \frac{3}{5}$. Q: Assuming we hadn't seen



how would we know if $\pi = \frac{3}{5}$ was a maximum or a minimum?

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This is **definitely negative**, so we have found the **maximum**.

First Derivative in R

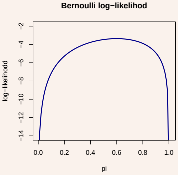
As shown above, the manual calculation is:

$$\begin{aligned}\frac{\partial \ln L(\pi|\boldsymbol{y})}{\partial \pi} &= \frac{\partial}{\partial \pi}[3\ln \pi + 2\ln(1-\pi)] \\ &= \frac{3}{\pi} + \frac{2}{1-\pi}\cdot(-1)\end{aligned}$$

<u>Note</u>: this can also be done in R using `deriv()`:

```
> deriv(f(x) ~ 3*log(x) + 2*log(1-x), "x")
expression({
    .expr3 <- 1 - x
    ...
    .grad[, "x"] <- 3 * (1/x) - 2 * (1/.expr3)
    ...
```

Second Derivative for Bernoulli Example in Detail



$$
\begin{aligned}
\frac{\partial^2 \ln L(\pi|\boldsymbol{y})}{\partial \pi^2} &= \frac{\partial}{\partial \pi}\left[\frac{3}{\pi} + \frac{2}{1-\pi} \cdot (-1)\right] \\
&= -\frac{3}{\pi^2} - \frac{2}{(1-\pi)^2} \\
&= -\frac{3}{.6^2} - \frac{2}{(1-.6)^2} \\
&= -20.83.
\end{aligned}
$$

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Optimization

The previous example we just developed is an example of **optimization**: the process of minimizing or maximizing a function by systematically choosing the values of variables from within an allowed set. For example:

$$\min_{x \in [-\infty, \infty]} f(x) = -\frac{1}{2}(3 - x)^2$$

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Two ways to solve:

1. analytically (we just did this using derivatives)
2. numerically (we'll do this in a minute)

Analytical Optimization: Univariate Case

Step One: Take the first derivative of the function and identify the critical value(s).

- The derivative of a function at a value x_0, denoted by $f'(x_0)$ or $\frac{\partial f}{\partial x}(x_0)$, is the instantaneous rate of change in $f(\cdot)$ at x_0.

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- It partially describes the behavior of a function on an interval [a,b]
  - If $f^{'}(x) > 0$ for all $x \in [a, b]$, then f is increasing on the interval $[a, b]$
  - If $f^{'}(x) < 0$ for all $x \in [a, b]$, then f is decreasing on the interval $[a, b]$
  - If $f^{'}(x) = 0$ at some $x \in [a, b]$ then we say x is a critical value of f. Critical values may be maxima, minima, or saddle points.

Analytical Optimization: Univariate Case

Step Two: Compute the second derivative of the function at the critical value(s) and evaluate.

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- The second derivative of a function $f''(x)$ or $\frac{\partial^2 f}{\partial x \partial x}(x)$ is the derivative of the derivative, or the rate of change of the rate of change.
- Use the following to evaluate your critical value(s):
  - If $f'(x_0) = 0$, and $f''(x_0) < 0$, then x_0 is a maximum
  - If $f'(x_0) = 0$ and $f''(x_0) > 0$, then x_0 is a minimum
  - If $f'(x_0) = 0$ and $f''(x_0) = 0$, then x_0 may be a minimum, a maximum, or neither.

Skip to numerical optimization

Analytical Optimization: Univariate Case

For example:

- Find extreme value of: $f(x) = x^3 - 3x^2$
- $f'(x) = 3x^2 - 6x = 3x(x-2)$ so $f'(x) = 0$ for $x = 0$ and $x = 2$.

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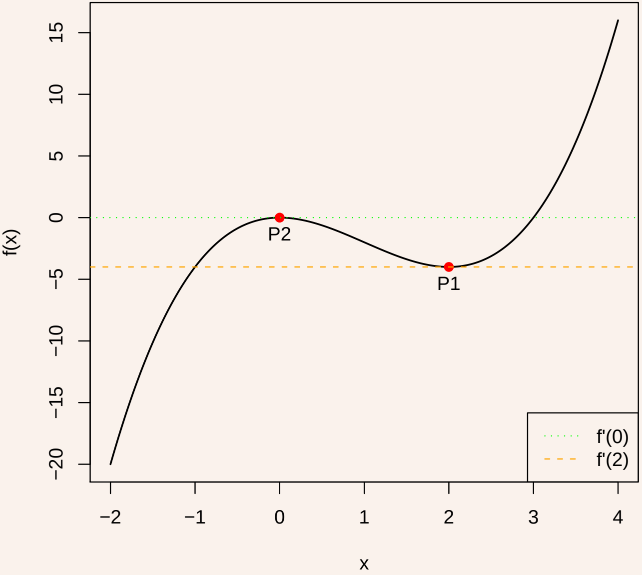
- Second derivative test: $f''(x) = 6x - 6 = 6(x-1)$
- Evaluate second derivative at critical values:
  - $f''(2) = 6$ so P_1 will be a minimum
  - $f''(0) = -6$ so P_2 will be a maximum


f(x)
x
P2
P1
f'(0)
f'(2)
−20
−15
−10
−5
0
5
10
15
−2
−1
0
1
2
3
4

Numerical Optimization

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There are a number of functions in R which can be used to optimize functions, but the one we will use most heavily is `optim()`.

Numerical Optimization Example

`optim()` takes a starting value (`par`) and a function (`fn`) as its main arguments.

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ll <- function(pie) return(3*log(pie) + 2*log(1-pie))

optim(par = .3, fn = ll, control = list(fnscale = -1),
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optim(par = .3, fn = ll, control = list(fnscale = -1),
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```

What are these three extra arguments?

1. `fnscale` multiplies the function by the given constant. As a default `optim()` finds the minimum so multiplying our function by -1 fools `optim()` into finding the maximum.
2. `method` is the variety of algorithm used to find the maximum. More on this in a second.
3. `hessian = TRUE` requests that `optim` return a matrix of second derivatives which in the above case will be 1x1.

Numerical Optimization Example Cont.

```
$par
[1] 0.6000034

$value
[1] -3.365058
...
$hessian
          [,1]
[1,] -20.83365

$Warning messages:
1: In log(1 - x) : NaNs produced
2: In log(1 - x) : NaNs produced
```

What is `optim` doing?

It depends on your choice in the `method` argument.

- `Nelder-Mead`: this is the default; it is slow but somewhat robust to non-differentiable functions.
- `BFGS`: a quasi-Newton Method; it is fast but needs a well behaved objective function.
- `L-BFGS-B`: similar to BFGS but allows box-constraints (i.e. upper and lower bounds on variables).
- `CG`: conjugate gradient method, may work for really large problems (we won't really use this).
- `SANN`: uses simulated annealing – a stochastic global optimization method; it is very robust but *very* slow.

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Our goal is to find move from x_0 to x_1 such that $f'(x_1) = 0$ (or is at least closer to 0 then than at x_0). This will be a sequential process of

approximation and eventually $f'(x_n)$ will be close enough to zero to let us declare that x_n a critical value.

Taylor Series Expansion: A Staple of Calculus

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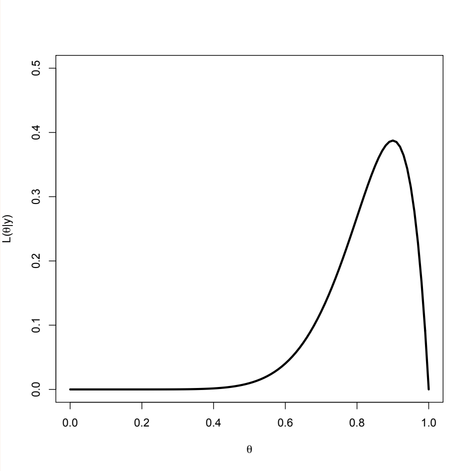
▸ Skip to multivariate optimization

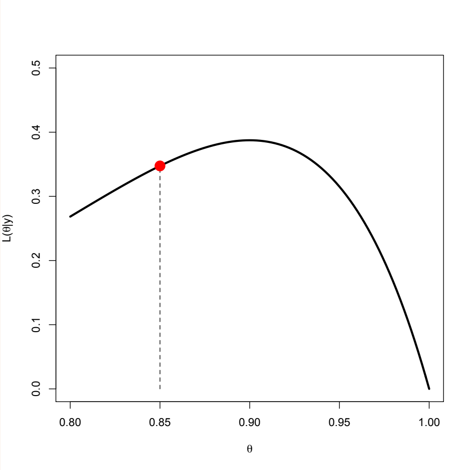
Likelihood of Binomial Distribution

This is the likelihood of a binomial distribution with 10 trials ($N = 10$) from which we drew one observation: $y = 9$.



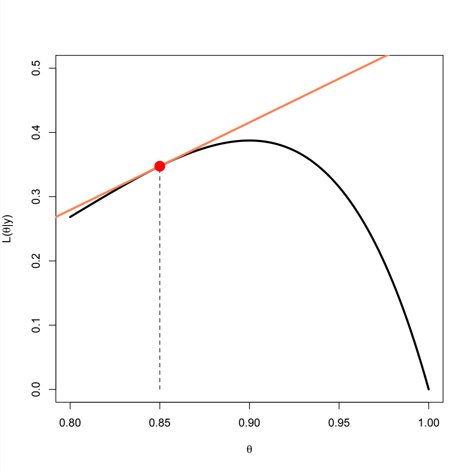
Likelihood of Binomial Distribution: Zoomed In

We want to approximate the likelihood curve around $\theta_0 = 0.85$.



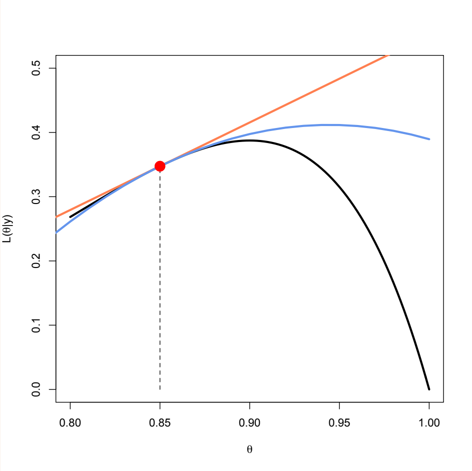
Likelihood of Binomial Distribution: Zoomed In

We can approximate the likelihood around $\theta_0 = 0.85$ using a first-order Taylor polynomial.



Likelihood of Binomial Distribution: Zoomed In

We can improve our approximation of the likelihood around $\theta_0 = 0.85$ by using a second-order Taylor polynomial.



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$$f'(\theta) = f'(\theta_0) + f''(\theta_0)(\theta - \theta_0) = 0$$

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$$f'(\theta) = f'(\theta_0) + f''(\theta_0)(\theta - \theta_0) = 0$$

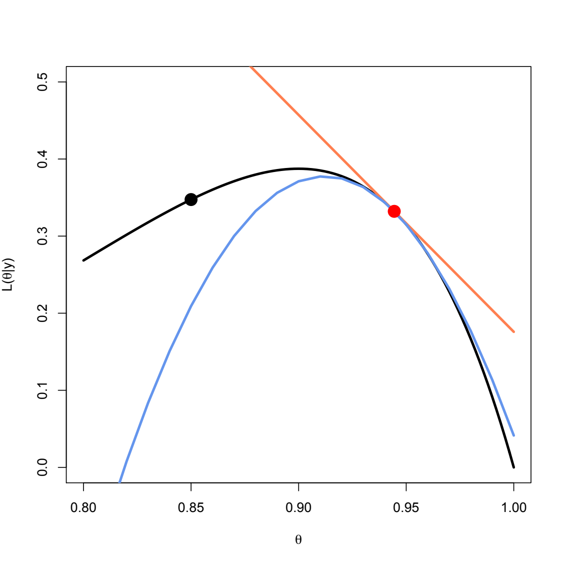
Rearranging:

$$\theta = \theta_0 - \frac{f'(\theta_0)}{f''(\theta_0)}$$

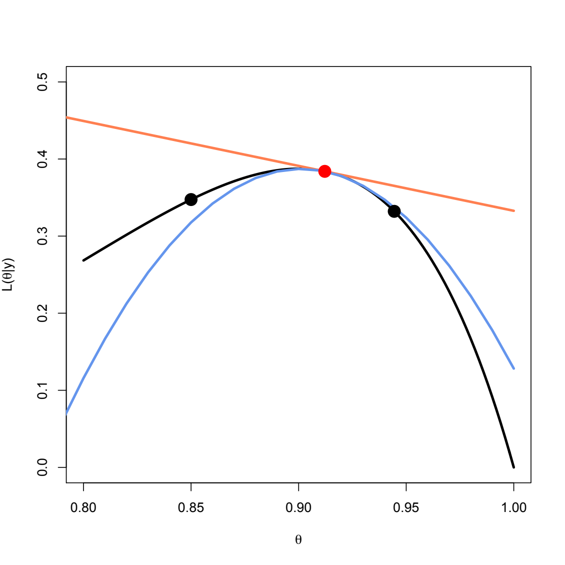
We've Just Derived the Update Step We Wanted!

$$\boxed{\theta_{n+1} = \theta_n - \frac{f'(\theta_n)}{f''(\theta_n)}}$$

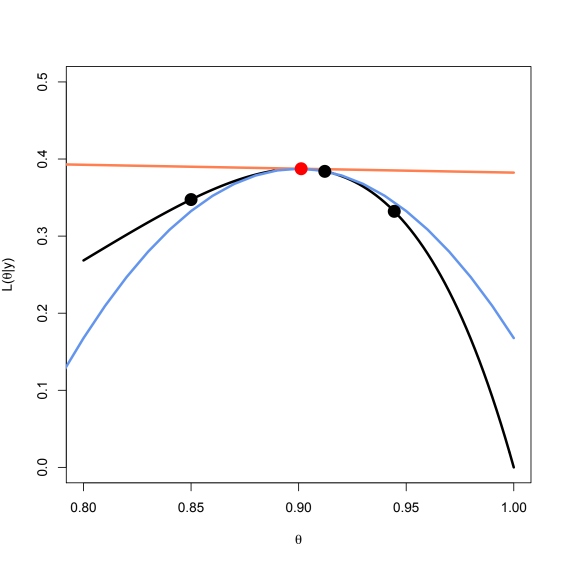
First Iteration



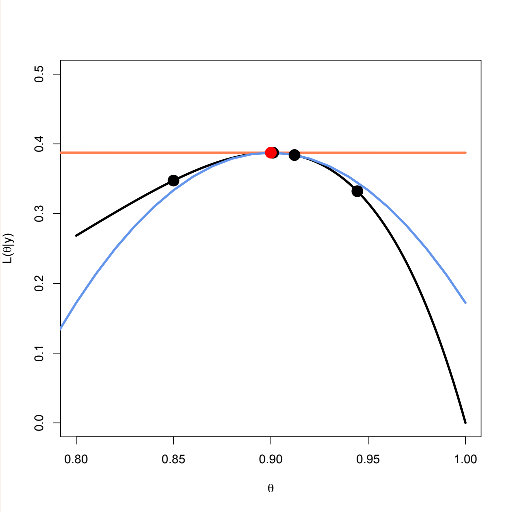
Second Iteration



Third Iteration



Fourth Iteration



Skip to Newton-Raphson properties
Skip to multivariate optimization

Another Example of Taylor Series Approximation

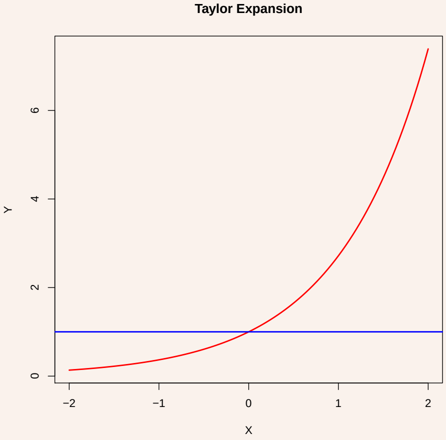


Figure : The exponential function, $g(x) = e^x$, and the Taylor Series approximation: $x_0 = 0$, $g_0(x_1) = 1$ (from Wikipedia)

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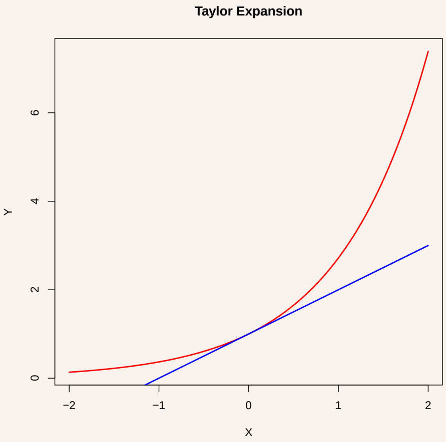

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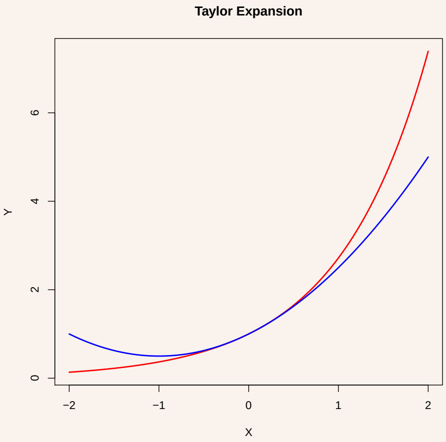

Figure : The exponential function, $g(x) = e^x$, and the Taylor Series approximation: $x_0 = 0, g_2(x_1) = 1 + x_1 + \frac{x^2}{2}$ (from Wikipedia)

Another Example of Taylor Series Approximation

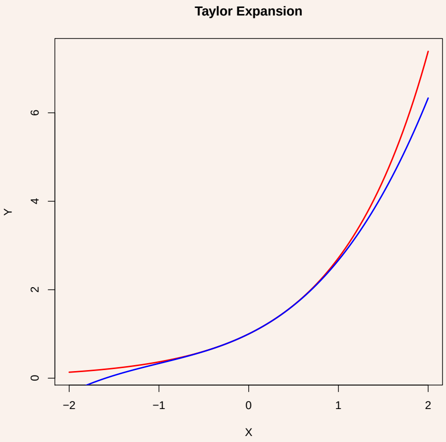

Figure : The exponential function, $g(x) = e^x$, and the Taylor Series approximation: $x_0 = 0$, $g_3(x_1) = 1 + x_1 + \frac{x^2}{2} + \frac{x^3}{6}$ (from Wikipedia)

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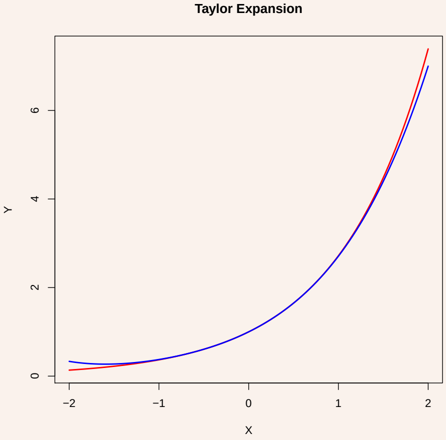

Figure : The exponential function, $g(x) = e^x$, and the Taylor Series approximation: $x_0 = 0$, $g_4(x_1) = 1 + x_1 + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24}$ (from Wikipedia)

Newton in Action: Bernoulli Example Revisited

Let's maximize our likelihood: $3 \ln \pi + 2 \ln(1 - \pi)$.

Recall that $L'(\pi) = \frac{3}{\pi} - \frac{2}{1-\pi}$ and $L''(\pi) = -\frac{3}{\pi^2} - \frac{2}{(1-\pi)^2}$.

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Starting at $\pi_0 = .3$, we use our updating formula:

$$\pi_1 = \pi_0 - \frac{L'(\pi_0)}{L''(\pi_0)} = .3 - \frac{L'(.3)}{L''(.3)} = 0.4909.$$

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Now use $\pi_1 = .4909$ as a starting value.

$$\pi_2 = \pi_1 - \frac{L'(\pi_1)}{L''(\pi_1)} = .4909 - \frac{L'(.4909)}{L''(.4909)} = 0.5991.$$

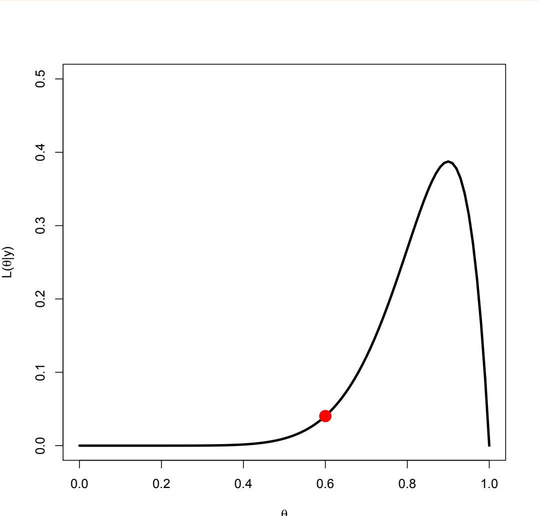
So we're already there!

Properties of Newton-Raphson

- Converges quickly
- Can get stuck in local minima/maxima
- Can have troubles with root jumping
- Won't walk at all on a flat space

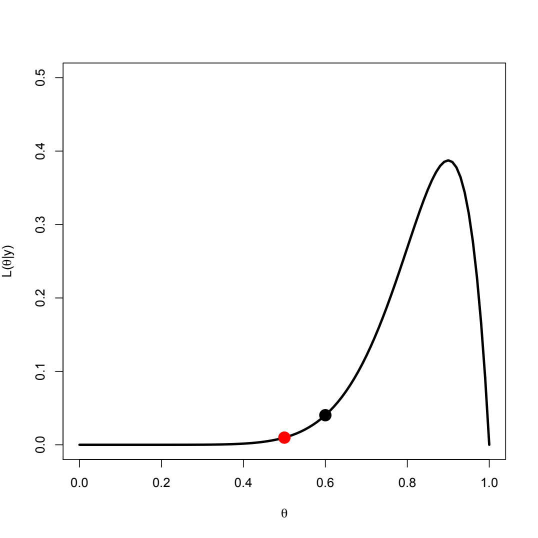
Newton-Raphson Gone Awry

What if we had taken $\theta_0 = 0.60$ to be the starting point for the Newton-Raphson maximization for the binomial likelihood?



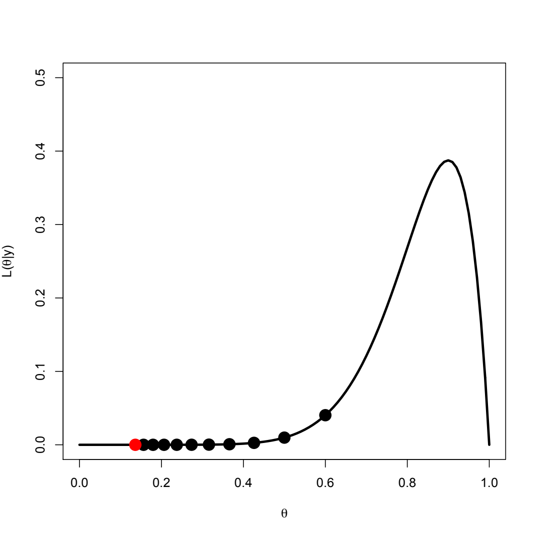
It Walks the Wrong Way...

The first iteration:



And Then Gets Stuck!

After 10 iterations:



Outline

The Multivariate Normal

Suppose I give you two observations (x=2, y=4) and tell you that they are from a bivariate normal distribution. It's known that $\sigma_x = \sigma_y = 1$ and x and y are uncorrelated. The two unknown parameters are μ_x and μ_y. The pdf is:

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So what's the likelihood?

$$L(\mu_x, \mu_y|x, y) \propto \frac{1}{2\pi} e^{-\frac{1}{2}\left[(x-\mu_x)^2+(y-\mu_y)^2\right]}.$$

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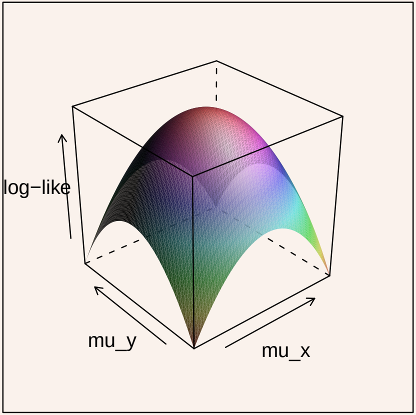
And the log-likelihood is especially nice:

$$\begin{aligned}\ln L(\mu_x, \mu_y|x, y) &\propto \ln\frac{1}{2\pi} - \frac{1}{2}\left[(x-\mu_x)^2 + (y-\mu_y)^2\right] \\ &\doteq -\frac{1}{2}\left[(x-\mu_x)^2 + (y-\mu_y)^2\right]\end{aligned}$$

Visualizing the Likelihood

We can plug in the datum and plot the likelihood:



▸ Skip to numerical optimization of multivariate normal
▸ Skip to full example of optimization

Multivariable Case: Analytically

Find extrema of:

$$\ell(\mu_x, \mu_y | x, y) \quad \propto \quad -\frac{1}{2}\left[(x - \mu_x)^2 + (y - \mu_y)^2\right]$$

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- $\frac{\partial \ell}{\partial \mu_y} = 4 - \mu_y$ is 0 if $\mu_y = 4$.
- So we have a critical value at $(\mu_x = 2, \mu_y = 4)$.

Multivariable Case: Analytically

Step Two: Evaluate critical value using the second derivative, but we have a wrinkle here because we have two variables. We're going to end up with a 2x2 Hessian matrix.

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$$H = \begin{pmatrix} \frac{\partial^2 l}{\partial \mu_x \partial \mu_x}(2,4) = -1 & \frac{\partial^2 l}{\partial \mu_x \partial \mu_y}(2,4) = \;\; 0 \\ \frac{\partial^2 l}{\partial \mu_y \partial \mu_x}(2,4) = \;\; 0 & \frac{\partial^2 l}{\partial \mu_y \partial \mu_y}(2,4) = -1 \end{pmatrix}$$

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It turns out that the key issue here for determining whether we have a maximum settles on whether the Hessian matrix is negative or positive definite (or something else). Define $a = \binom{a_1}{a_2}$.

1. negative definite: $a'Ha < 0$ for all $a \neq 0 \rightarrow$ maximum.
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Our example is easy: $a'Ha = (-a_1 \quad -a_2)\binom{a_1}{a_2} = -a_1^2 - a_2^2$. So we're **negative definite**.

Multivariate Case: Numerically

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```
ll <- function(par){
  mux <- par[1]
  muy <- par[2]
  like <- -.5*((2-mux)^2+(4-muy)^2)
  return(like)
}

optim(par = c(0,0), fn = ll, method = "BFGS",
      control = list(fnscale = -1), hessian = TRUE)
```

```
$par
[1] 2 4

$value
[1] -4.930381e-31
...
$convergence
[1] 0
...
$hessian
              [,1]          [,2]
[1,] -1.000000e+00 -2.646978e-17
[2,] -2.646978e-17 -1.000000e+00
```

Skip to full example of optimization

optim() Techniques in Practice

You can always test these techniques on some function.

```
fkt <- function(x){10*sin(0.3*x)*sin(1.3*x^2)
                   + 0.00001*x^4 + 0.2*x+80}
```

Figure : Plotting the Wild Function

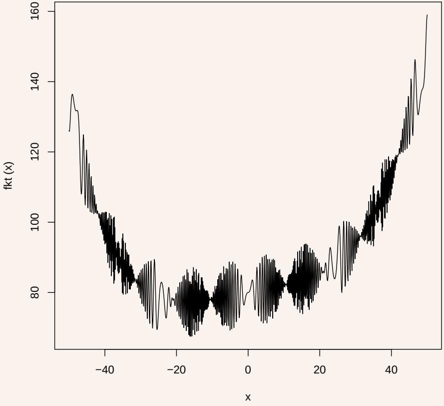
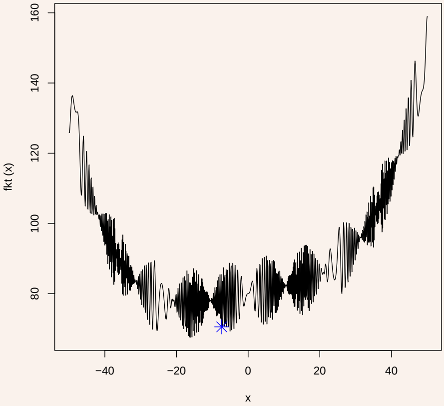
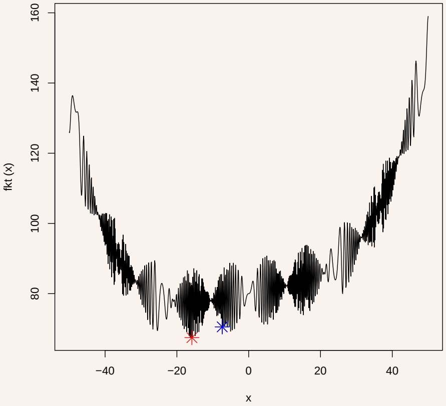


Figure : Using BFGS at x=50




```
out <- optim(par = 50, fkt, method="BFGS",
             control=list(maxit=20000, parscale=20))
points(out$par, out$val, pch = 8, col="blue", cex=2)
```

Figure : Using Simulated Annealing at x=50




```
out <- optim(par = 50, fkt, method="SANN",
             control=list(maxit=20000, temp=20, parscale=20))
points(out$par, out$val, pch = 8, col = "red", cex = 2)
```

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Putting It All Together

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We want to find λ, which is the mean of the Poisson distribution.

The PMF (discrete) for the data is

$$p(\boldsymbol{y}|\lambda) = \prod_{i=1}^{n} \frac{\lambda^{y_i} e^{-\lambda}}{y_i!}$$

Since $L(\theta|\boldsymbol{y}) \propto p(\boldsymbol{y}|\theta)$, we have

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$$\ell(\lambda|\boldsymbol{y}) \quad = \quad \sum_{i=1}^{n} (y_i \ln \lambda) - n\lambda$$

Why Can We Use the Log-likelihood?

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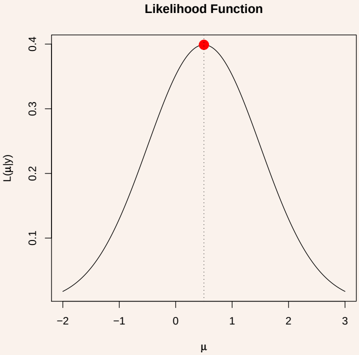

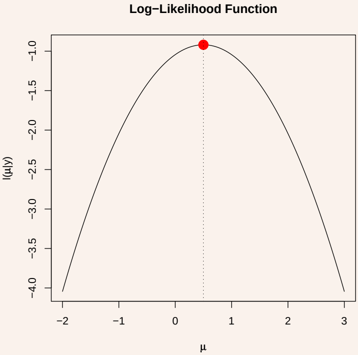

Skip to finding MLE in R

Finding the Maximum Likelihood Estimate (MLE)

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$$\begin{aligned} \frac{\partial \ell(\lambda|\boldsymbol{y})}{\partial \lambda} = S(\lambda) &= \frac{\sum_{i=1}^{n} y_i}{\lambda} - n \\ 0 &= \frac{\sum_{i=1}^{n} y_i}{\lambda} - n \end{aligned}$$

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0 &= \frac{\sum_{i=1}^{n} y_i}{\lambda} - n \\
\hat{\lambda} &= \frac{\sum_{i=1}^{n} y_i}{n}
\end{aligned}$$

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```
> ll.poisson <- function(par, y) {
+     lambda <- exp(par)
+     out <- sum(y * log(lambda)) - length(y) * lambda
+     return(out)
+ }
```

Maximum Likelihood In R

Find the maximum (with sample data):

```
> data <- rpois(1000, 5)
> opt <- optim(par = 2, fn = ll.poisson, method = "
    BFGS", control = list(fnscale = -1),
+       y = data)$par
> mle <- exp(opt)
> mle
```

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```

```
[1] 4.996001
```