MTH3045: Statistical Computing

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Week 6 lecture 1

Challenges I

- Go to Challenges I of the week 6 lecture 1 challenges at https://byoungman.github.io/MTH3045/challenges

Sherman-Morrison formula / Woodbury matrix identity

- In general, unless we actually need the inverse of a matrix (such as for standard errors of regression coefficients in a linear model), we should solve systems of linear equations
- Sometimes, though, we do need – or might just have – an inverse, and want to calculate something related to it
- The following are a set of formulae, which go by various names, that can be useful in this situation

Woodbury's formula

- Consider an $m \times m$ matrix $\mathbf{A}$, with m large, and for which we have the inverse, $\mathbf{A}^{-1}$
- Suppose $\mathbf{A}$ receives a small update of the form $\mathbf{A} + \mathbf{U}\mathbf{V}^\mathsf{T}$, for $m \times n$ matrices $\mathbf{U}$ and $\mathbf{V}$ where $n \ll m$
- Then, by **Woodbury's formula**,

$$(\mathbf{A} + \mathbf{U}\mathbf{V}^\mathsf{T})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{U}(\mathbf{I}_n + \mathbf{V}^\mathsf{T}\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}^\mathsf{T}\mathbf{A}^{-1}$$

- *Remark*: What's important to note here is that we're looking to calculate an $m \times m$ inverse with m large, and so in general this will be an $O(m^3)$ calculation based on the LHS
- However, in the above, the RHS only requires that we to invert an $n \times n$ matrix, at cost $O(n^3)$, which is much less that of the LHS, if we already have $\mathbf{A}^{-1}$.

Sherman-Morrison-Woodbury formula

- Woodbury's formula above generalises to the so-called **Sherman-Morrison-Woodbury formula** by introducing the $n \times n$ matrix $\mathbf{C}$, so that

$$(\mathbf{A} + \mathbf{U}\mathbf{C}\mathbf{V}^{\mathsf{T}})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{U}(\mathbf{C}^{-1} + \mathbf{V}^{\mathsf{T}}\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}^{\mathsf{T}}\mathbf{A}^{-1}$$

Challenges II

- Go to Challenges II of the week 6 lecture 1 challenges at https://byoungman.github.io/MTH3045/challenges

Sherman-Morrison formula

- The **Sherman-Morrison formula** is the special case of Woodbury's formula (and hence the Woodbury-Sherman-Morrison formula) in which the update to $\mathbf{A}$ can be considered in terms of m-vectors $\mathbf{u}$ and $\mathbf{v}$, so that

$$(\mathbf{A} + \mathbf{u}\mathbf{v}^\mathsf{T})^{-1} = \mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{u}\mathbf{v}^\mathsf{T}\mathbf{A}^{-1}}{1 + \mathbf{v}^\mathsf{T}\mathbf{A}^{-1}\mathbf{u}}$$

- *Remark*: The Sherman-Morrison formula is particularly useful because it requires no matrix inversion

Example: Bayesian linear regression I

- Recall from MTH2006 the normal linear model where

$$Y_i \sim N(\mathbf{x}_i^\mathsf{T}\beta, \sigma^2)$$

  with independent errors $\varepsilon_i = Y_i - \mathbf{x}_i^\mathsf{T}\beta$s, for $i = 1, \ldots, n$, where $\mathbf{x}_i^\mathsf{T} = (1, x_{i1}, \ldots, x_{ip})$ is the ith row of design matrix $\mathbf{X}$ and where $\boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_p)^\mathsf{T}$
- Hence

$$\mathbf{Y} \mid \mathbf{X}\beta \sim MVN_n(\mathbf{X}\beta, \sigma^2\mathbf{I}_n)$$

- In Bayesian linear regression, the elements of β and σ^2 are not fixed, unknown parameters: they are random variables, and we must declare *a priori* our beliefs about their distribution
- The conjugate prior is that

$$\boldsymbol{\beta} \sim MVN_{p+1}(\boldsymbol{\mu}_{\boldsymbol{\beta}}, \boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1})$$

- Integrating out β gives

$$\mathbf{Y} \sim MVN_n(\mathbf{X}\boldsymbol{\mu}_{\boldsymbol{\beta}}, \sigma^2\mathbf{I}_n + \mathbf{X}\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1}\mathbf{X}^\mathsf{T})$$

Example: Bayesian linear regression II

- Now suppose that we want to evaluate the marginal likelihood for an observation, $\mathbf{y}$, say. Recall the MVN pdf
- The Mahalanobis distance then involves the term

$$(\mathbf{y} - \mathbf{X}\boldsymbol{\mu}_{\boldsymbol{\beta}})^{\mathsf{T}}(\sigma^2 \mathbf{I}_n + \mathbf{X}\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1}\mathbf{X}^{\mathsf{T}})^{-1}(\mathbf{y} - \mathbf{X}\boldsymbol{\mu}_{\boldsymbol{\beta}})$$

- The covariance of the marginal distribution, $\sigma^2 \mathbf{I}_n + \mathbf{X}\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1}\mathbf{X}^{\mathsf{T}}$, is typically dense, expensive to form, and leads to expensive solutions to systems of linear equations
- Its inverse, however, can be computed through the Sherman-Morrison-Woodbury formula with $\mathbf{A}^{-1} = \sigma^{-2}\mathbf{I}_n$, $\mathbf{U} = \mathbf{V} = \mathbf{X}$, and $\mathbf{C} = \boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1}$

Bibliographic notes

- For more details on matrix decompositions, consider Wood (2015, Appendix B) for a concise overview
- For fuller details consider Monahan (2011, chaps. 3, 4 and 6) or Press et al. (2007, chap. 2 and 11)

Chapter 4: Numerical Calculus

Numerical Calculus: Motivation

- In statistics, we often rely on the Normal distribution with pdf

$$\phi(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$

  and cdf

$$\Phi(x; \mu, \sigma^2) = \int_{-\infty}^{x} \phi(x; \mu, \sigma^2) \mathrm{d}x.$$

- Unfortunately no closed form exists for $\Phi(x; \mu, \sigma^2)$
- However, if x, μ and σ are stored in `R` as `x`, `mu` and `sigma`, we can still evaluate $\Phi(x; \mu, \sigma^2)$ with `pnorm(x, mu, sigma)`
- This is one example of a frequently-occurring situation in which we somehow want to evaluate an intractable integral
- This raises the question: are there generic methods that let us evaluate intractable integrals?
- The answer is often **numerical integration**

Numerical Calculus: Motivation

- *Remark*: In this chapter, we'll consider generic methods for integration, i.e. that work in many scenarios
- Sometimes, such as evaluating $\Phi(x; \mu, \sigma^2)$, specific algorithms will give more accurate results
- This is what `R` does for `pnorm()`

Numerical Differentiation

- In Chapter 5 we will cover optimisation of functions, such as numerically finding maximum likelihood estimates when analytical solutions aren't available
- We'll see that supplying derivatives can considerably improve estimation, typically in terms of reducing computation time
- Here we'll cover some useful results in terms of differentiation of matrices, which will later prove useful
- No knowledge of analytical matrix calculus beyond these results will be needed for MTH3045
- The matrix cookbook (Petersen and Pedersen 2012), however, can provide you with a much more thorough set of differentiation rules, should you ever need them

Differentiation definitions I

- **Definition**: Consider $f : \mathbb{R}^n \to \mathbb{R}$, which we'll consider a function of vector $\mathbf{x} = (x_1, \ldots, x_n)^\mathsf{T}$
- The **gradient operator**, ∇, is defined as

$$\nabla f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{pmatrix}$$

- Note that in MTH3045 we will have no cause to consider multivariate functions, i.e. to consider $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$, for $m > 1$

Differentiation definitions II

- **Definition**: Consider again $f : \mathbb{R}^n \to \mathbb{R}$
- The **Hessian matrix** is the matrix of second derivatives of f, whereas the gradient operator considered first derivatives, and is given by

$$\nabla^2 f(\mathbf{x}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

- The Hessian matrix plays an important role in statistics, in particular for estimating parameter uncertainty via the Fisher information, which is covered in MTH3028
- In the next chapter, we'll also see that it's important for optimisation

Differentiation rules I

- Now consider $g : \mathbb{R}^n \to \mathbb{R}$ a function of $\mathbf{x}$ that, for fixed $\mathbf{A}$, takes the quadratic form $g(\mathbf{x}) = \mathbf{x}^\mathsf{T}\mathbf{A}\mathbf{x}$ for $n \times n$ matrix $\mathbf{A}$ and n-vector $\mathbf{x}$
- Then
$$\nabla g(\mathbf{x}) = (\mathbf{A} + \mathbf{A}^\mathsf{T})\mathbf{x} \quad \text{and} \quad \nabla^2 g(\mathbf{x}) = \mathbf{A} + \mathbf{A}^\mathsf{T}$$
- Note that in the case of symmetric $\mathbf{A}$, $\nabla g(\mathbf{x}) = 2\mathbf{A}\mathbf{x}$ and $\nabla^2 g(\mathbf{x}) = 2\mathbf{A}$

Differentiation rules II

- Next consider $h : \mathbb{R}^n \to \mathbb{R}$ a function of n-vector $\mathbf{x}$ and p-vector $\mathbf{y}$ that, for fixed $n \times n$ matrix $\mathbf{A}$ and $n \times p$ matrix $\mathbf{B}$, takes the quadratic form $h(\mathbf{x}, \mathbf{y}) = (\mathbf{x} + \mathbf{B}\mathbf{y})^{\mathsf{T}}\mathbf{A}(\mathbf{x} + \mathbf{B}\mathbf{y})$
- Then

$$\frac{\partial h(\mathbf{x}, \mathbf{y})}{\partial \mathbf{x}} = (\mathbf{A} + \mathbf{A}^{\mathsf{T}})(\mathbf{x} + \mathbf{B}\mathbf{y}) \quad \text{and} \quad \frac{\partial h(\mathbf{x}, \mathbf{y})}{\partial \mathbf{y}} = \mathbf{B}^{T}(\mathbf{A} + \mathbf{A}^{\mathsf{T}})(\mathbf{x} + \mathbf{B}\mathbf{y}),$$

  and also

$$\frac{\partial^2 h(\mathbf{x}, \mathbf{y})}{\partial \mathbf{x} \partial \mathbf{x}^{\mathsf{T}}} = \mathbf{A} + \mathbf{A}^{\mathsf{T}} \quad \text{and} \quad \frac{\partial^2 h(\mathbf{x}, \mathbf{y})}{\partial \mathbf{y} \partial \mathbf{y}^{\mathsf{T}}} = \mathbf{B}^{\mathsf{T}}(\mathbf{A} + \mathbf{A}^{\mathsf{T}})\mathbf{B}$$

- Note that above we use partial derivative notation, i.e. ∂, as opposed to gradient operator notation, i.e. ∇, as the derivatives are not w.r.t. all variables.

Challenges III

- Go to Challenges III of the week 6 lecture 1 challenges at https://byoungman.github.io/MTH3045/challenges

Week 6 lecture 2

Example: Maximum likelihood estimates of regression coefficients in the normal linear model via matrix calculus I

- Consider the normal linear model $\mathbf{Y} = \mathbf{X}\beta + \boldsymbol{\varepsilon}$
  - $\mathbf{Y} = (Y_1, \ldots, Y_n)^\mathsf{T}$
  - $\mathbf{X}$ is an $n \times (p+1)$ design matrix
  - β is a $(p+1)$-vector of regression coefficients
  - $\boldsymbol{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_n)^\mathsf{T}$ with independent $\varepsilon_i \sim N(0, \sigma^2)$
- The maximum likelihood estimate of β, denoted $\hat{\beta}$, minimises the RSS, i.e. minimises

$$(\mathbf{y} - \mathbf{X}\beta)^\mathsf{T}(\mathbf{y} - \mathbf{X}\beta)$$

  if we observe $\mathbf{y} = (y_1, \ldots, y_n)^\mathsf{T}$
- Differentiating w.r.t. β gives

$$-\mathbf{X}^\mathsf{T}(\mathbf{y} - \mathbf{X}\beta) - (\mathbf{y} - \mathbf{X}\beta)^\mathsf{T}\mathbf{X}$$

Example: Maximum likelihood estimates of regression coefficients in the normal linear model via matrix calculus II

- Then
$$-\mathbf{X}^\mathsf{T}(\mathbf{y}-\mathbf{X}\beta)-(\mathbf{y}-\mathbf{X}\beta)^\mathsf{T}\mathbf{X}$$
simplifies to
$$-2\mathbf{X}^\mathsf{T}(\mathbf{y}-\mathbf{X}\beta)$$
as $\mathbf{X}^\mathsf{T}(\mathbf{y}-\mathbf{X}\beta)$ and $(\mathbf{y}-\mathbf{X}\beta)^\mathsf{T}\mathbf{X}$ are both n-vectors
- The derivative of the RSS is zero at $\hat{\beta}$ and so
$$-2\mathbf{X}^\mathsf{T}(\mathbf{y}-\mathbf{X}\hat{\beta})=0$$
- Therefore $\hat{\beta}$ is the solution of
$$\mathbf{X}^\mathsf{T}\mathbf{X}\hat{\beta}=\mathbf{X}^\mathsf{T}\mathbf{y}$$
- Alternatively
$$\hat{\beta}=(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$
as we were given in MTH2006

Finite-differencing

- Consider again $f(\mathbf{x})$, a function of vector $\mathbf{x}$
- **Definition**: Consider $f : \mathbb{R}^n \to \mathbb{R}$ for n-vector $\mathbf{x}$
- Let, $\mathbf{e}_i$ be the n-vector comprising entirely zeros, except for its ith element, which is one
- Then the **partial derivative** of $f(\mathbf{x})$ w.r.t. x_i, the ith element of $\mathbf{x}$, is

$$\frac{\partial f(\mathbf{x})}{\partial x_i} = \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{e}_i) - f(\mathbf{x})}{h}$$

- The preceding definition leads us to the **finite-difference** partial derivative approximation

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \simeq \frac{f(\mathbf{x} + \delta\mathbf{e}_i) - f(\mathbf{x})}{\delta},$$

where δ is small

Example: Finite-differencing of $\sin(x)$ I

- Use finite-differencing to approximate the derivative of $f(x) = \sin(x)$ for $x \in [0, 2\pi]$, and compare its accuracy to the true derivative
- First, let's calculate f and its *true* derivative, i.e. $f'(x) = \cos(x)$, and store this as `partial0` for $\{x_i\}$, $i = 1, \ldots, 100$, a set of equally-spaced points on $[0, 2\pi]$

```r
n <- 100
x <- seq(0, 2 * pi, l = 100)
f <- sin(x)
partial0 <- cos(x)
```

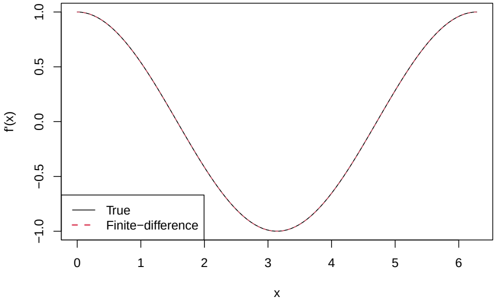
- Now we'll set $\delta = 10^{-6}$ and calculate $x_i + \delta$, for each x_i, i.e. each element of `x`, so that the finite-difference approximation to the derivative is given by $[\sin(x_i + 10^{-6}) - \sin(x_i)]/10^{-6}$, which is calculated below and stored as `partial1`

```r
delta1 <- 1e-6
x1 <- x + delta1
f1 <- sin(x1)
partial1 <- (f1 - f) / delta1
```

Example: Finite-differencing of sin(x) II

- We'll then plot the $f'(x)$ against it finite-difference approximation

```r
matplot(x, cbind(partial0, partial1), type = 'l', xlab = 'x', ylab = "f'(x)")
legend('bottomleft', lty = 1:2, col = 1:2, lwd = 1:2,
       legend = c('True', 'Finite-difference'))
```



- In fact, the true derivative and its finite-difference approximation are so similar that's it's difficult to distinguish the two, but they're both there in the plot!

Example: Finite-differencing of sin(x) III

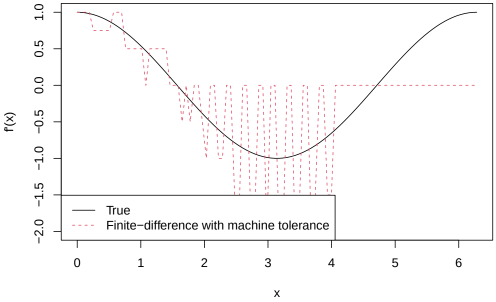
- We might be tempted to choose δ as small as possible
- Suppose we were to repeat Example 4.3 with $\delta = \epsilon_m$, i.e. R's machine tolerance
- The following calculates the finite-difference approximation as `partial2`

```r
delta2 <- .Machine$double.eps
x2 <- x + delta2
f2 <- sin(x2)
partial2 <- (f2 - f) / delta2
```

Example: Finite-differencing of $\sin(x)$ III

- The the following plots this against the true value of $f'(x)$

```
matplot(x, cbind(partial0, partial2), type = 'l', xlab = 'x', ylab = "f'(x)")
legend('bottomleft', lty = 1:2, col = 1:2, bg = 'white',
       legend = c('True', 'Finite-difference with machine tolerance'))
```



- Using $\delta = \epsilon_m$ gives a terrible approximation to $f'(x)$, which gets worse as x increases
- We've actually encountered an example *calculation error*, which was introduced in Chapter 2

Challenges I

- Go to Challenges I of the week 6 lecture 2 challenges at https://byoungman.github.io/MTH3045/challenges

Example: Finite differencing of the multivariate Normal log-likelihood I

- Find $\partial \log f(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) / \partial y_i$ analytically, for $i = 1, \ldots, p$, where $f(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$ is the $MVN_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ pdf, for arbitrary $\mathbf{y}$, $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$
- Evaluate this for $\mathbf{y}$, $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ as in Example 3.2
- Then approximate the same derivative using finite-differencing
- The logarithm of the $MVN_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ pdf is given by

$$\log f(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{1}{2} \left[p \log(2\pi) + \log(|\boldsymbol{\Sigma}|) + (\mathbf{y} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu}) \right]$$

  which we know, from Example 3.13, we can evaluate with `dmvn3()`

- Using the above properties

$$\frac{\partial \log f(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})}{\partial \mathbf{y}} = -\boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu})$$

  since $\boldsymbol{\Sigma}$ is symmetric

Example: Finite differencing of the multivariate Normal log-likelihood II

- We can evaluate this for $\mathbf{y}$, $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ as in Example 3.2 with the following

  ```
  y <- c(.7, 1.3, 2.6)
  mu <- 1:3
  Sigma <- matrix(c(4, 2, 1, 2, 3, 2, 1, 2, 2), 3, 3)
  deriv1 <- -solve(Sigma, y - mu)
  ```

  which gives

  ```
  as.vector(deriv1)
  ```

  ```
  ## [1] -0.08  0.38 -0.14
  ```

Example: Finite differencing of the multivariate Normal log-likelihood III

- To approximate the derivative by finite-differencing, it makes sense to write a multi-purpose function for finite differencing, which we'll call `fd()`

```r
fd <- function(x, f, delta = 1e-6, ...) {
  # Function to evaluate derivative w.r.t. vector by finite-differencing
  # x is a p-vector
  # fn is the function for which the derivative is being calculated
  # delta is the finite-differencing step, which defaults to 10^{-6}
  # returns a vector of length x
  f0 <- f(x, ...)
  p <- length(x)
  f1 <- numeric(p)
  for (i in 1:p) {
    ei <- replace(numeric(p), i, 1)
    f1[i] <- f(x + delta * ei, ...)
  }
  (f1 - f0) / delta
}
```

Example: Finite differencing of the multivariate Normal log-likelihood IV

- Then we can use this with `dmvn3()` with the following

  ```
  deriv2 <- fd(y, dmvn3, mu = mu, Sigma = Sigma)
  ```

  which gives

  ```
  deriv2
  ```

  ```
  ## [1] -0.0800002  0.3799993 -0.1400008
  ```

  and is the same as the analytical result

  ```
  all.equal(deriv1, deriv2)
  ```

  ```
  ## [1] "Mean relative difference: 2.832689e-06"
  ```

  once we allow for error in the finite-difference approximation

Challenges II

- Go to Challenges II of the week 6 lecture 2 challenges at https://byoungman.github.io/MTH3045/challenges

Week 6 lecture 3

Quadrature

- Another common requirement in statistics is that some integral needs to be evaluated
- To start, let's consider a simple integral of the form

$$I = \int_a^b f(x)\mathrm{d}x$$

- We'll first take a look at some *deterministic* approaches to numerically evaluating integrals
- In fact, these all boil down to assuming that

$$I \simeq \sum_{i=1}^{N} w_i f(x_i^*)$$

  for some weights w_i and nodes x_i^*, $i = 1, \ldots, N$
- Note that here we're considering the so-called *composite* approach to approximating an interval, i.e. in which a rule is applied over a collection of sub-intervals

Midpoint rule

- Perhaps the first numerical integration scheme we come across is the midpoint rule
- Put simply, we divide $[a, b]$ into N equally-sized intervals, and use the midpoints of these as the nodes, x_i^*
- This gives

$$\int_a^b f(x)\mathrm{d}x \simeq h \sum_{i=1}^{N} f(x_i^*),$$

  where $x_i^* = a + (i - 0.5)(b - a)/N$ and $h = (b - a)/N$
- The error in the approximation is $O(h^2)$
- Thus more intervals reduces h and gives a more accurate approximation
- We can measure accuracy through **relative absolute error**
- **Definition**: The **relative absolute error**, or sometimes just *relative error*, of an estimate of some true value is given by

$$\left| \frac{\text{true value} - \text{estimate}}{\text{true value}} \right|$$

Example: Midpoint rule I

- Consider the integral $\int_0^1 \exp(x)\mathrm{d}x = \exp(1) - 1 \simeq 1.7182818$
- Use R and the midpoint rule to estimate the integral with $N = 10$, 100 and 1000
- Then compare the relative absolute error of each
- We'll start by calculating the true value of the integral, which we'll store as `true`

```r
true <- exp(1) - 1
```

- Then we'll store the values of N that we're testing as `N_vals`

```r
N_vals <- 10^c(1:3)
```

Example: Midpoint rule II

- The following then creates a vector, `midpoint`, in which to store the integral approximations, and calculates the approximations with a `for` loop
- Inside the loop the integration nodes (i.e. the midpoints) and h are calculated

```r
midpoint <- numeric(length(N_vals))
for (i in 1:length(N_vals)) {
  N <- N_vals[i]
  nodes <- (1:N - .5) / N
  h <- 1 / N
  midpoint[i] <- h * sum(exp(nodes))
}
midpoint
```

```
## [1] 1.717566 1.718275 1.718282
```

Example: Midpoint rule III

- The relative absolute error for each is then given in the vector `rel_err_mp` below

```
rel_err_mp <- abs((true - midpoint) / true)
rel_err_mp
```

```
## [1] 4.165452e-04 4.166655e-06 4.166667e-08
```

- We clearly see that the absolute error reduces by two factors of ten for each factor of ten increase in N, which is consistent with the above comment of $O(h^2)$ error, where here $h = 1/N$

Challenges III

- Go to Challenges III of the week 6 lecture 2 challenges at https://byoungman.github.io/MTH3045/challenges

Simpson's rule

- The midpoint rule works simply by approximating $f(x)$ over a sub-interval of $[a, b]$ by a horizontal line
- The trapezium rule (which we'll overlook) assumes a straight line
- Simpson's rule is derived from a quadratic approximation and given by

$$\int_a^b f(x)\mathrm{d}x \simeq \frac{h}{6}\left(f(a) + 4\sum_{i=1}^{N} f(x_{1i}^*) + 2\sum_{i=1}^{N-1} f(x_{2i}^*) + f(b)\right),$$

  where $x_{1i}^* = a + h(2i-1)/2$, $x_{2i}^* = a + ih$ and $h = (b-a)/N$
- Note that Simpson's rule requires $N + 1$ more evaluations of f than the midpoint rule
  - however, a benefit of those extra evaluations is that its error reduces to $O(h^4)$

Example: Simpson's rule I

- Now use `R` and Simpson's rule to approximate the integral $\int_0^1 \exp(x)\mathrm{d}x = \exp(1) - 1$ with $N = 10$, 100 and 1000, compare the relative absolute error for each, and against those of the midpoint rule in Example 4.5
- We already have `true` and `N_vals` from Example 4.5, and we can use a similar `for` loop to approximate the integral using Simpson's rule
- The main difference is that we create two sets of nodes, `nodes1` and `nodes2`, which correspond to the x_{1i}s and x_{2i}s in Equation (4.1), respectively

Example: Simpson's rule II

- The integral approximations are stored as `simpson`

```r
simpson <- numeric(length(N_vals))
N_vals <- 10^c(1:3)
for (i in 1:length(N_vals)) {
  N <- N_vals[i]
  h <- 1 / N
  simpson[i] <- 1 + exp(1)
  nodes1 <- h * (2*c(1:N) - 1) / 2
  simpson[i] <- simpson[i] + 4 * sum(exp(nodes1))
  nodes2 <- h * c(1:(N - 1))
  simpson[i] <- simpson[i] + 2 * sum(exp(nodes2))
  simpson[i] <- h * simpson[i] / 6
}
print(simpson, digits = 12)
```

```
## [1] 1.71828188810 1.71828182847 1.71828182846
```

- We print this to 11 decimal places so we can see where the approximations changes with N

Example: Simpson's rule III

- Finally we calculate the relative absolute errors, `rel_err_simp`,

```r
rel_err_simp <- abs((true - simpson) / true)
rel_err_simp
```

```
## [1] 3.471189e-08 3.472270e-12 6.461239e-16
```

- We see a dramatic improvement in the accuracy of approximation that Simpson's rule brings, with relative absolute errors of the same order of magnitude as those form the midpoint rule using $N = 1000$ achieved with $N = 10$ for Simpson's rule
- Note, though, that for given N, Simpson's rule requires $N + 1$ more evaluations of $f()$

Challenges I

- Go to Challenges I of the week 6 lecture 3 challenges at https://byoungman.github.io/MTH3045/challenges

Gaussian quadrature I

- We've seen that Simpson's rule can considerably improve on the midpoint rule for approximating integrals
- However, we might still consider both restrictive in that they consider an equally-spaced set of nodes
- **Definition**: Consider $g(x)$, a polynomial of degree $2N-1$, and a fixed weight function $w(x)$
- Then, the **Gauss-Legendre quadrature rule** states that

$$\int_a^b w(x)g(x)\mathrm{d}x = \sum_{i=1}^{N} w_i g(x_i),$$

where, for $i = 1, \ldots, N$, w_i and x_i depend on $w(x)$, a and b, but not $g(x)$

Gaussian quadrature II

- The Gauss-Legendre quadrature rule is the motivation for **Gaussian quadrature**, whereby we assume that the integral we're interested in can be well-approximated by a polynomial
- This results in the approximation

$$\int_a^b f(x)\mathrm{d}x \simeq \sum_{i=1}^N w_i f(x_i)$$

  for a fixed set of x values, x_i with corresponding weights w_i, for $i = 1, \ldots, N$
- There are many rules for choosing the weights, w_i, but (perhaps fortunately) we won't go into them in detail in MTH3045
- Instead, we'll just consider the function `pracma::gaussLegendre()` (for which you'll need to install the `pracma` package), where `pracma::gaussLegendre(N, a, b)` produces `N` nodes and corresponding weights on the interval [a,b], with $N =$ `N`, $a =$ `a` and $b =$ `b`

Gaussian quadrature III

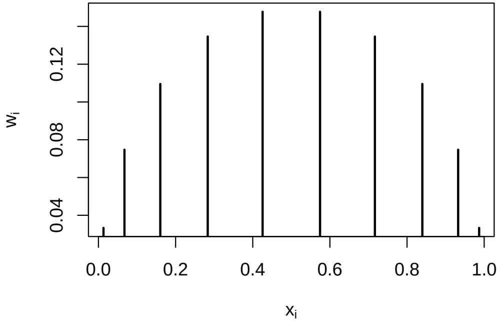
- The following produces nodes and weights for $N = 10$ on $[0, 1]$

```
gq <- pracma::gaussLegendre(10, 0, 1)
gq
```

```
## $x
##  [1] 0.01304674 0.06746832 0.16029522 0.28330230 0.42556283 0.57443717
##  [7] 0.71669770 0.83970478 0.93253168 0.98695326
##
## $w
##  [1] 0.03333567 0.07472567 0.10954318 0.13463336 0.14776211 0.14776211
##  [7] 0.13463336 0.10954318 0.07472567 0.03333567
```

Gaussian quadrature IV

- The plots below shows the nodes and their weights



- The nodes are spread further apart towards the middle of the $[0, 1]$ range, but given more weight
- Note that `pracma::gaussLegendre()` is named so because it implements Gauss-Legendre quadrature, i.e. Gaussian quadrature with Legendre polynomials[1]

[1]Wikipedia has a useful pages on Gaussian quadrature and on Legendre polynomials, should you want to read more on them

Example: Gaussian quadrature I

- Now use R and Gauss-Legendre quadrature to approximate the integral $\int_0^1 \exp(x) \mathrm{d}x$ with $N = 10$
- Explore what value of N gives a comparable estimate to that of the midpoint rule with $N = 100$ based on relative absolute error
- We can re-use true from Example 4.5 and then we'll consider $N = 10$, 4 and 3, which we'll call N_vals, and store the resulting integral approximations in gauss.

```r
N_vals <- c(10, 4, 3)
gauss <- numeric(length(N_vals))
for (i in 1:length(N_vals)) {
  N <- N_vals[i]
  xw <- pracma::gaussLegendre(N, 0, 1)
  gauss[i] <- sum(xw$w * exp(xw$x))
}
gauss
```

```
## [1] 1.718282 1.718282 1.718281
```

Example: Gaussian quadrature II

- The relative absolute errors, `rel_err_gauss`,

  ```
  rel_err_gauss <- abs((true - gauss) / true)
  rel_err_gauss
  ```

  ```
  ## [1] 2.584496e-16 5.429651e-10 4.795992e-07
  ```

  show that, having considered $N = 3, 4, 10$, choosing $N = 3$ for Gaussian quadrature gives closest relative absolute error to that of the midpoint rule with $N = 100$, which really is quite impressive
- Note, though, that $f(x) = \exp(x)$ is a very smooth function
  - for wiggler functions, larger N is likely to be needed, and improvements in performance, such as Gaussian quadrature over the midpoint rule, might be significantly less

Challenges II

- Go to Challenges II of the week 6 lecture 3 challenges at

  https://byoungman.github.io/MTH3045/challenges

Example: Poisson marginal approximation using Gaussian quadrature I

- Consider a single random variable $Y \mid \lambda \sim \text{Poisson}(\lambda)$, where we can characterise our prior beliefs about λ as $\lambda \sim \text{N}(\mu, \sigma^2)$
- Use Gaussian quadrature with $N = 7$ to estimate the marginal pdf of Y if $\mu = 10$ and $\sigma = 3$
- The marginal pdf of Y is given by

$$f(y) = \int_{-\infty}^{\infty} f(y \mid \lambda) f(\lambda) \mathrm{d}\lambda$$

- *Remark*: The *three sigma rule* is a heuristic rule of thumb that 99.7% of values lie within three standard deviations of the mean

Example: Poisson marginal approximation using Gaussian quadrature II

- Hence for the $N(10, 3^2)$ distribution we should expect 99.7% of values to lie within $10 \pm 3 \times 3$
- Hence we'll take this as our range for the Gaussian quadrature nodes.

```
mu <- 10
sigma <- 3
N <- 7  # no. of nodes
xw <- pracma::gaussLegendre(
        N,
        mu - 3 * sigma, # left-hand end
        mu + 3 * sigma # right-hand end
)
xw
```

```
## $x
## [1]  1.458029  3.326219  6.347394 10.000000 13.652606 16.673781 18.541971
##
## $w
## [1] 1.165365 2.517349 3.436470 3.761633 3.436470 2.517349 1.165365
```

which are stored as `xw$x` with corresponding weights `xw$w`, $w_1, \ldots, w_N$

Example: Poisson marginal approximation using Gaussian quadrature III

- Next we want a set of values at which to evaluate $f(y)$, and for this we'll choose $0, 1, \ldots, 30$, which we can create in R with

```
y_vals <- 0:30
```

- Then we can estimate $f(y)$ as

$$\hat{f}(y) \simeq \sum_{i=1}^{N} w_i f(y \mid \lambda_i^*) f(\lambda_i^*)$$

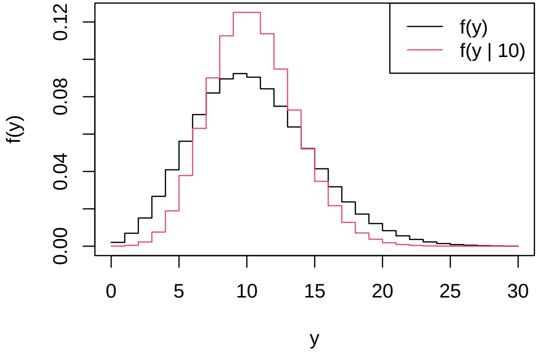
- The following code gives $\hat{f}(y)$ as fhat for y in the set of values y_vals

```
m <- length(y_vals)
fhat <- numeric(m)
for (i in 1:m) {
  fhat[i] <- sum(xw$w * dpois(y_vals[i], xw$x) *
                   dnorm(xw$x, mu, sigma))
}
```

Example: Poisson marginal approximation using Gaussian quadrature IV

- Finally, we'll plot $\hat{f}(y)$ against the pdf of the Poisson(10) distribution

```r
matplot(y_vals, cbind(fhat, dpois(y_vals, mu)), lwd = 1,
        col = 1:2, lty = 1, type = 'l', xlab = 'y', ylab = 'f(y)')
legend('topright', c("f(y)", "f(y | 10)"),
       lty = 1, col = 1:2)
```



- $f(y)$ is broader than $f(y \mid 10)$, which is to be expected given that $f(y)$ integrates out the variability in λ given by the $\mathrm{N}(10, 3^2)$ distribution

One-dimensional numerical integration in `R`

- Unsurprisingly, `R` has a function for one-dimensional numerical integration
- It's called `integrate()`
- It uses a method that builds on Gaussian quadrature, but we won't go into its details
- Use of `integrate()`, however, is fairly straightforward

Example: Integration with `integrate()`

- Evaluate the integral $\int_0^1 \exp(x)dx = \exp(1) - 1$ using `R`'s `integrate()` function with $N = 10$ and report its relative absolute error
- We can use the following code, where the first argument to `integrate()` is the function we're integrating, the second and third are the lower and upper ranges of the definite integral, and `subdivisions` is the maximum number of nodes to use in the approximation, which defaults to 100.

```r
true <- exp(1) - 1
estimate <- integrate(function(x) exp(x), 0, 1, subdivisions = 10)
estimate
```

```
## 1.718282 with absolute error < 1.9e-14
```

```r
rel_err <- abs((true - estimate$value) / true)
rel_err
```

```
## [1] 1.292248e-16
```

- Note above that the absolute error is similarly tiny to that of Gaussian quadrature above
- The values themselves, being so close to the machine tolerance, are incomparable
    - but we can be sure that the approximation is incredibly accurate

References

Monahan, John F. 2011. *Numerical Methods of Statistics*. 2nd ed. Cambridge University Press. https://doi.org/10.1017/CBO9780511977176.

Petersen, K. B., and M. S. Pedersen. 2012. *The Matrix Cookbook*. https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf.

Press, W. H., S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. 2007. *Numerical Recipes: The Art of Scientific Computing*. 3rd ed. Cambridge University Press. https://books.google.co.uk/books?id=1aAOdzK3FegC.

Wood, Simon N. 2015. *Core Statistics*. Institute of Mathematical Statistics Textbooks. Cambridge University Press. https://doi.org/10.1017/CBO9781107741973.