Computational Skills for Biostatistics I: Lecture 7

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Algorithms

This lecture is intended to give a very fast and broad overview of some common algorithms in statistics

- Matrix inversion
- Newton-Raphson
- Gradient descent
- Linear programs
- Monte Carlo integration
- Markov Chain Monte Carlo
- Metropolis Hastings
- Hamiltonian Monte Carlo

Every single one of these topics could be a quarter-long course

Thanks

Many thanks to Mauricio Sadinle, Dan Kowal, Noah Simon, Mike Betancourt, Mark Schmidt, and many others for resources used to make these slides

How do we compare algorithms

- Arithmetic complexity: number of arithmetic operations it takes to run an algorithm

Computational complexity

Example: How many arithmetic operations does it take to multiply two $n \times n$ matrices: $C = AB$

$$c_{ij} = \begin{bmatrix} a_{i1}, a_{i1}, \ldots, a_{in} \end{bmatrix} \begin{bmatrix} b_{1j} \\ b_{2j} \\ \vdots \\ b_{nj} \end{bmatrix} = \sum_{h=1}^{n} a_{ih} b_{hj}$$

Computational complexity

Example: How many arithmetic operations does it take to multiply two $n \times n$ matrices: $C = AB$

For each (i, j) we do n multiplications and $n - 1$ sums

We need $n^2(2n - 1)$ arithmetic operations (fewer operations if we know the structure!)

Big O notation

Goal: to describe asymptotic behaviour of a function

How do the computational requirements of the algorithm grow as a function of the input?

Big O notation

Example. Say your algorithm takes $f(n)$ arithmetic operations, e.g.

$$f(n) = \log(n) + 6n + 4n^2$$

Big O notation

Example. Say your algorithm takes $f(n)$ arithmetic operations, e.g.

$$f(n) = \log(n) + 6n + 4n^2$$

As n grows, the dominant term in the sum is n^2 (even the constant becomes irrelevant when $n \to \infty$)

The fastest growing term determines the order of $f(n)$

Big O notation

Definition. We say $f(n) = O(g(n))$ if and only if there exists a constant $M > 0$ and a real number n_0 such that

$$|f(n)| \leq M|g(n)| \quad \text{for all} \quad n \geq n_0.$$

Big O notation

Where n is the size of a matrix:

- (Naive) matrix multiplication: $O(n^3)$
- (Naive) matrix inversion: $O(n^3)$

We can also talk about different inputs, e.g., magnitude of inputs in bits

Matrix inversion

Matrix inversion is extremely common in statistics
What is your favourite example?

Matrix inversion

We can write the least squares estimate as

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

or as the solution to

$$(X^T X)\beta = X^T Y$$

Which is faster?

General problem

- A : $n \times n$ full-rank matrix
- b : $n \times 1$ vector
- $z^* = A^{-1}b$: solution of system of linear equations $Az = b$

This **does not mean** that you should compute A^{-1} and then multiply by b

Matrix inversion

Fact: solving systems of equations is often faster (and never slower) than finding inverses

- If you can, avoid computing inverses!
- Instead, **just solve the system of linear equations** $Az = b$

Note: A^{-1} is the solution to $AZ = I_n$

If you can, avoid computing inverses!

Both solving $Az = b$ and computing A^{-1} by Gaussian elimination have arithmetic complexity of $O(n^3)$

While they have the same asymptotic complexity, solving $Az = b$ is much faster!

- **The big O notation can be misleading!**

Note: there exist faster algorithms than $O(n^3)$ for computing inverses but many are not practical for usual values of n

Practical implementation in R

```
solve( t(X) %*% X ) # find inverse
solve( t(X) %*% X, t(X) %*% Y ) # solve (X^TX)\beta=X^TY
```

Regression example

```r
X <- replicate(2000, rnorm(10000)); Y <- rnorm(10000)
system.time( b1 <- solve( t(X) %*% X ) %*% t(X) %*% Y )
```

```
##    user  system elapsed
##  52.780   0.405  53.798
```

```r
system.time( b2 <- solve( t(X) %*% X,
                          t(X) %*% Y ) )
```

```
##    user  system elapsed
##  24.487   0.160  24.926
```

```r
sum((b1 - b2)^2)
```

```
## [1] 1.172123e-29
```

Regression example

```
ops <- function(h){ Xh <- X[,1:h]
 t1 <- system.time( solve( t(Xh) %*% Xh ) %*%
                      t(Xh) %*% Y )[3]
 t2 <- system.time( solve( t(Xh) %*% Xh,
                           t(Xh) %*% Y ) )[3]
 data.frame("inverse" = t1, "solve" = t2)
}
ps <- seq(from = 50, to = 300, by = 50)
times <- sapply(ps, ops)
colnames(times) <- paste("p =", ps)
```

Regression example

```
times
```

```
##          p = 50 p = 100 p = 150 p = 200 p = 250 p = 300
## inverse 0.037  0.126   0.275   0.469   0.726   1.065
## solve   0.015  0.064   0.141   0.254   0.396   0.552
```

About twice as fast to solve a linear system!

Matrix inversion

Conclusions

- avoid if possible
- solve systems instead
- used closed form solution for special cases (e.g., diagonal, block)

Algorithms

- ~~Matrix inversion~~
- Newton-Raphson
- Gradient descent
- Linear programs
- Monte Carlo integration
- Markov Chain Monte Carlo
- Metropolis Hastings
- Hamiltonian Monte Carlo

Newton Raphson

Goal: Solve $f(x) = 0$

Idea: Taylor expand around x_n:

$$f(x) \approx f(x_n) + f'(x_n)(x - x_n)$$

then solve for $f(x) = 0$:

$$x = x_n - \frac{f(x_n)}{f'(x_n)}$$

Newton Raphson

Goal: Solve $f(x) = 0$

Algorithm: start at reasonable guess x_0, then set

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Pros: easy, converges quickly

Cons: needs smooth functions and first derivatives

Newton Raphson: finding stationary points

Goal: Solve $f'(x) = 0$

Algorithm: start at reasonable guess x_0, then set

$$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$$

or for multivariate functions,

$$x_{n+1} = x_n - [\nabla^2 f|_{x_n}]^{-1} \nabla f|_{x_n}$$

Newton Rapson: finding stationary points

Goal: Solve $f'(x) = 0$

Common modification:

$$x_{n+1} = x_n - \gamma[\nabla^2 f|_{x_n}]^{-1}[\nabla f|_{x_n}]$$

for $\gamma \in (0, 1)$

- Pros: more stable
- Cons: slower

Gradient descent

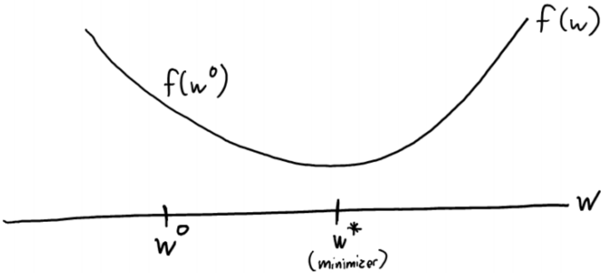
Goal: minimise $f(x)$

Algorithm: move in the steepest direction

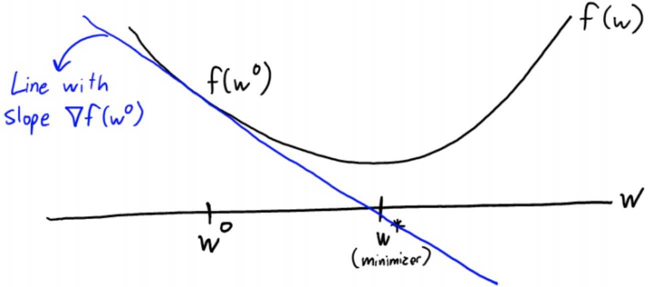
$$x_{n+1} = x_n - \gamma \nabla f(x_n)$$

for small γ

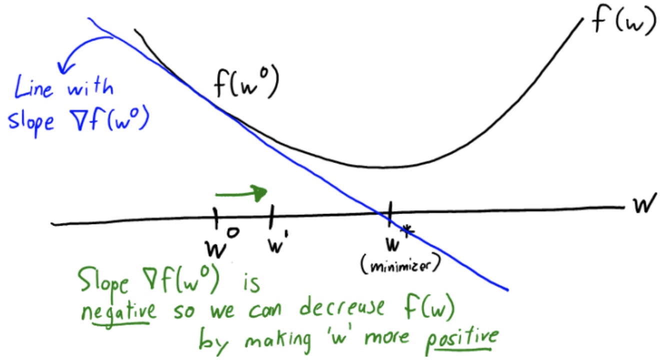
Gradient descent



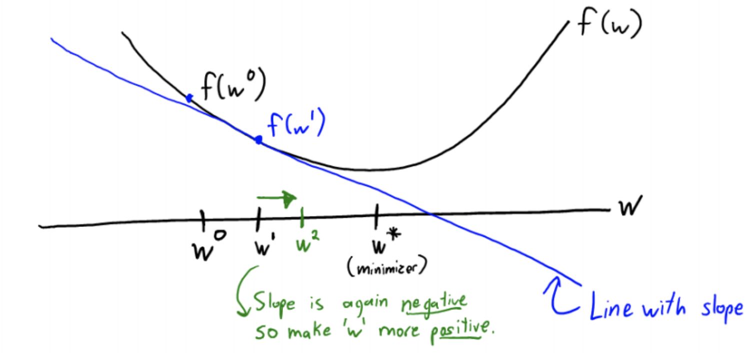
Gradient descent



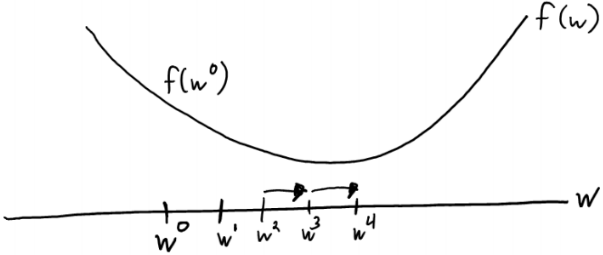
Gradient descent


f(w)
f(w^0)
Line with slope $\nabla f(w^0)$
w
w^0
w^1
w^*
(minimizer)
Slope $\nabla f(w^0)$ is negative so we can decrease f(w) by making 'w' more positive

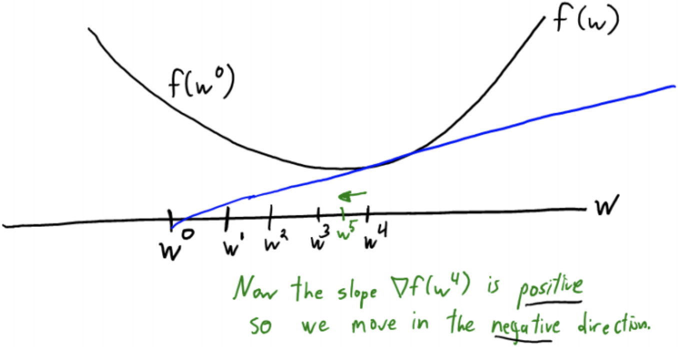
Gradient descent



Gradient descent



Gradient descent



Now the slope $\nabla f(w^4)$ is positive so we move in the negative direction.

Gradient descent

Also called steepest descent

- Pros
  - Don't use second derivatives (curvature)
  - Don't need to take an inverse
  - Guarantees exist for convex functions
- Cons
  - Theoretically not as fast

Linear programming

Goal: Solve a linear objective function with linear constraints

Minimise $c^T x$ subject to $Ax \leq b$ and $x \geq 0$

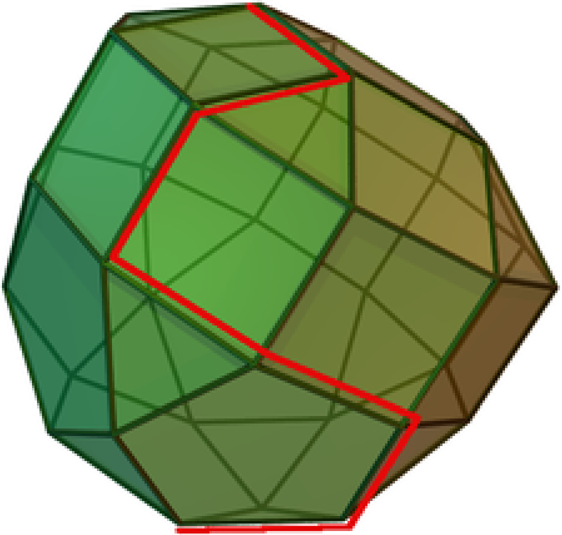
Related: Linear integer programming

Linear programming

Minimise $c^T x$ subject to $Ax \leq b$ and $x \geq 0$

- Solution exists on boundary of convex polytope
- Common algorithm: Simplex algorithm
- Exponential at worst case but typically outperforms provably better algorithms in practice

Simplex Algorithm



Algorithms

- ~~Matrix inversion~~
- ~~Newton-Raphson~~
- ~~Gradient descent~~
- ~~Linear programs~~
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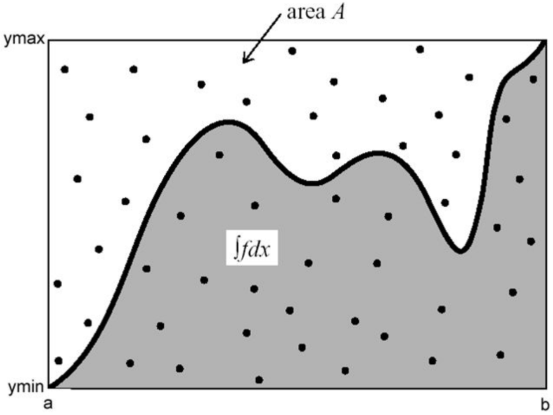
Monte Carlo

Monte Carlo typically refers to a numerical integration procedure



Monte Carlo

Monte Carlo methods are extremely common in Bayesian statistics where it is difficult to obtain the posterior distribution in closed form

That is, we can't maximise the posterior distribution directly because we can't even write it down!

Monte Carlo

However, we don't often care about finding the posterior distribution – typically we care about functions of the posterior

- moments
    - mean
    - variance
- quantiles

Most functions of the posterior can be written as integrals – hence, Monte Carlo integration

Monte Carlo

Problem: Find $\int_{\mathbb{R}^k} g(x)f(x)dx$ for integrable g

Setting: we can simulate from $f(x)$

Algorithm: Draw $X_1, \ldots, X_n \overset{iid}{\sim} f$ and estimate $\int_{\mathbb{R}^k} g(x)f(x)dx$ by $\frac{1}{N}\sum_{i=1}^{N} g(X_i)$

By the law of large numbers, this is a consistent estimator

Monte Carlo

Challenge: It's typically hard to get an iid sample from f

Markov chain Monte Carlo

Proposal: Create a Markov chain with stationary distribution f

Markov Chain: $f(X_{t+1}|X_0, \ldots, X_t) = f(X_{t+1}|X_t)$

How do we create such a Markov chain?

Markov Chain Monte carlo

Goal: Create a Markov chain with stationary distribution as posterior

Approaches:

- Metropolis sampling
    - Metropolis Hastings sampling
        - Gibbs sampling

Gibbs sampling

Idea: Break full posterior into product of conditionals

Algorithm:

- Partition posterior into blocks
  - $p(\theta_b|X, \theta_{-b}) = p(\theta_b|X, \theta_1, \ldots, \theta_{b-1}, \theta_{b+1}, \ldots, \theta_p)$
- Sample from blocks
  - Sample $\theta_1^s \sim p(\theta_1|X = x, \theta_{-1} = \theta^s_{-1})$
  - Sample $\theta_2^s \sim p(\theta_2|X = x, \theta_{-2} = \theta^s_{-2})$
  - $\ldots$
  - Sample $\theta_p^s \sim p(\theta_p|X = x, \theta_{-p} = \theta^s_{-p})$
- For large enough s, θ^s is a draw from $p(\theta|X = x)$

Metropolis sampling

Problem: Generate a Markov chain with stationary distribution p

Setting: Can evaluate $\pi(\theta|x)$ for some π such that $p(\theta|x) \propto \pi(\theta|x)$

Want to sample from $p(\theta|x)$ (typically posterior) and
$p(\theta|x) \propto \pi(\theta|x)$ (typically unnormalised posterior)

Metropolis

Algorithm:

- Propose $Y \sim q(\cdot|X_t)$, where q is some *symmetric* proposal distribution
- Calculate acceptance probability

$$\alpha(X_t, Y) = min\left\{1, \frac{\pi(Y)}{\pi(X_t)}\right\}$$

  - If proposal increases density, take it
  - If proposal decreases density, take it with some probability
- Let $X_{t+1} = Y$ with probability α and X_t otherwise.

This algorithm generates a Markov chain $X_0, X_1, X_2, \ldots$ with stationary distribution p

Metropolis *Hastings*

Algorithm:

- Propose $Y \sim q(\cdot|X_t)$, where q is some proposal distribution
- Calculate acceptance probability

$$\alpha(X_t, Y) = min\left\{1, \frac{\pi(Y)q(X_t|Y)}{\pi(X_t)q(Y|X_t)}\right\}$$

- Let $X_{t+1} = Y$ with probability α and X_t otherwise.

This algorithm generates a Markov chain $X_0, X_1, X_2, \ldots$ with stationary distribution f

Choosing proposal distributions

- There are many options for choosing the proposal distribution q.
- Proposal distribution not necessarily related to p or π
- A common choice is $q(\cdot|X) = \mathcal{N}(X, \sigma^2)$.

Problem with MH-MCMC

Problem: α is typically low

- Waste a lot of time generating proposals that are not accepted
- Problem exacerbated in high dimensional settings

Hamiltonian Monte Carlo

Problem: Generate a Markov chain with stationary distribution f

Algorithm/approach:

- Leverage physics of the problem (mass/momentum of distribution at current state)

Idea: Use Hamiltonian dynamics to more efficiently sample from f

Amazing resource: STAN

HMC via Stan

“Stan is a C++ library for Bayesian inference using the No-U-Turn sampler (a variant of Hamiltonian Monte Carlo) or frequentist inference via optimization.”

- RStan is the R interface to Stan

HMC via Stan

Classic example: Bayesian meta-analysis

- Observations are a noisy draw from true mean
  - $Y_j \sim N(\theta_j, \sigma_j^2)$
- Goal is to estimate mean of means μ
  - $\theta_j \sim N(\mu, \tau)$
- Y_j observed, σ_j^2 known
- μ, τ parameters

HMC via Stan

- See schools example
- Note: Stan is not R; it is its own language
  - An interface between the two exists

HMC via Stan

- Extremely easy! Basically no math is required to do Bayesian inference
- However, it's critical to know how to diagnose problems
  - Parametrisation
  - Convergence

Coming up

- Homework 7: due next *Wednesday*
  - Newton Raphson
  - Gradient descent
  - Stan
  - An algorithm of your choosing!