Gradient Methods

Julia Wrobel

Overview

Today, we cover:

- Review of GLMs
- Gradient methods
    - Newtons method continued
    - Iteratively reweighted least squares for GLM
    - Quasi-Newton

Announcements

- HW3 posted later today and due 3/4 at 10:00AM
- No class tomorrow, 2/12

Readings:

- Peng Chapter 3
- Givens and Hoeting Chapter 2

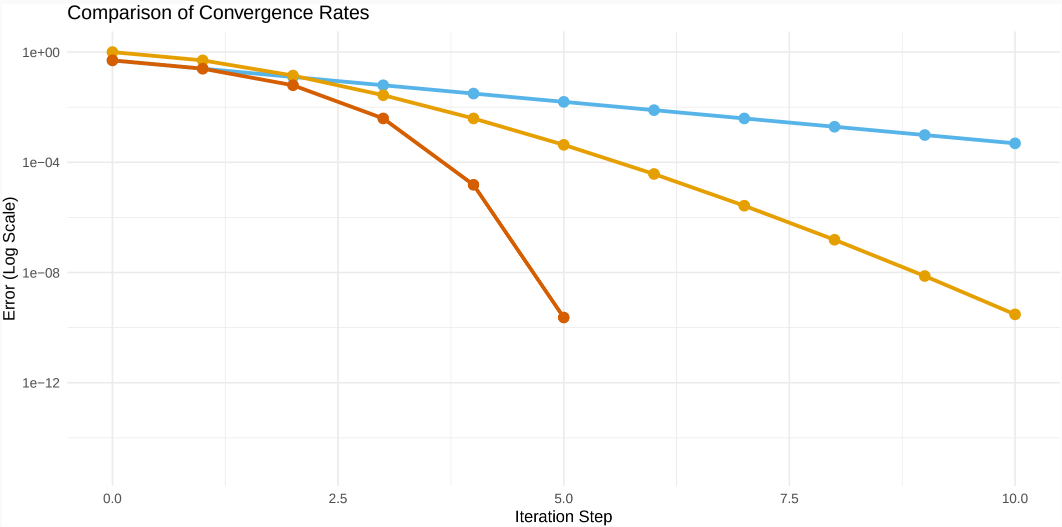
Rates of convergence

One of the ways algorithms can be compared is via their rates of convergence to some limiting value.

- Typically we have an iterative algorithm that is trying to find the max/min of an objective function f
    - Want to estimate how long it will take to reach that optimal value
- Three rates of convergence we will focus on:
    - **linear** (slowest)
    - **superlinear** (faster)
    - **quadratic** (fastest)

Algorithms that require more information about f (such as its derivative) tend to converge more quickly.

Rates of convergence



Generalized linear models (GLMs)

Extension of standard linear model to allow for non-Normal response distributions.

$$g(\mu_i) = x_i^T \beta \tag{1}$$

$$\mu_i = E(Y_i | x_i) \tag{2}$$

- $g(\cdot)$ is a known link function
- $Y_i \sim EF$, iid
    - Exponential Family distribution, i.e. Normal, binomial, Poisson, etc.
- $Var(Y_i | X_i) = \phi Var(\mu)$
    - Known variance function that (often) depends on the mean

Canonical links

Model	Normal	Poisson	Binomial	Gamma
ϕ	σ^2	1	$1/m$	$1/\nu$
$b(\theta)$	$\theta^2/2$	$\exp(\theta)$	$\log(1+e^\theta)$	$-\log(-\theta)$
μ	θ	$\exp(\theta)$	$e^\theta/(1+e^\theta)$	$-1/\theta$
Canonical link g	identity	$\log$	logit	reciprocal
Variance function V	1	μ	$\mu(1-\mu)$	μ^2

Generalized linear models (GLMs)

Linear regression:

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

GLMs:

- $\hat{\beta}$ (typically) cannot be obtained in closed form
- Need an numeric estimation approach, i.e. an **iterative algorithm**

Poisson regression

$$\log(E[Y_i|X_i]) = X_i^T\beta$$

- $Y_i \sim Poisson(\mu_i)$
- $Var(\mu_i) = \mu_i$
- $g'(\mu_i) = \frac{1}{\mu_i}$

How do we find β?

- Use maximum likelihood

Poisson regression log-likelihood

$$l(\mu_i) = \sum_i (y_i \log \mu_i - \mu_i - \log y_i!)$$

- $\mu_i = e^{X_i^T \beta}$

$$l(\beta) = \sum_i \left(y_i X_i^T \beta - e^{X_i^T \beta} - \log y_i! \right)$$

Estimate unknown β by solving

$$\hat{\beta} = \arg\min_{\beta} \sum_i \left(y_i X_i^T \beta - e^{X_i^T \beta} - \log y_i! \right)$$

Poisson regression log-likelihood

Can solve using steepest descent or Newton

- Need gradient and Hessian

- **gradient**: $\frac{\partial l(\beta)}{\partial \beta} = \sum_i (Y_i - e^{X_i^T \beta}) X_i$

- **Hessian**: $\frac{\partial^2 l(\beta)}{\partial \beta^2} = -\sum_i e^{X_i^T \beta} X_i^T X_i$

- **Is this a convex optimization problem?**

Poisson regression optimization

Using **Steepest Descent**:

$$\beta_{t+1} = \beta_t - \alpha \frac{\partial l(\beta)}{\partial \beta}$$

Using **Newton's Method**

$$\beta_{t+1} = \beta_t - \left[\frac{\partial^2 l(\beta)}{\partial \beta^2}\right]^{-1} \frac{\partial l(\beta)}{\partial \beta}$$

Exercise

Go to lab exercise, implement Newton's method for Poisson regression. Compare with result from `glm()`

Fisher's information

Sometimes, gradient and Hessian (or related quantities) go by other names in the context of statistical modeling.

- **Score function**: first derivative of log-likelihood with respect to parameter vector β. This is the gradient.

$$U(\beta) = \nabla \log L(\beta)$$

- **Information** (aka Fisher's information): negative expected value of the Hessian.

$$I(\beta) = Var[U(\beta)] = -E\left[\nabla^2 \log L(\beta)\right] = [Var(\beta)]^{-1}$$

- **observed information**: A function of the sample size n. Negative of the Hessian.

$$I_n(\theta) = -[\nabla^2 \log L(\theta)]_{\theta=\hat{\theta}}$$

Observed vs. Expected information

- Observed information is often easier to work with
- In many GLMs, observed and expected information are equivalent
- Expected information shown to outperform observed in constructing confidence intervals

Observed vs. Expected information: Poisson

Newton's method for GLMs

From last lecture, the Newton's method update is:

$$x_{t+1} = x_t - \{f''(x_t)\}^{-1} f'(x_t).$$

If you are trying to optimize parameters β in a log-likelihood function, this becomes:

$$\begin{aligned}
\beta_{t+1} &= \beta_t - \{l''(\beta_t)\}^{-1} l'(\beta_t) && (3)\\
&= \beta_t + \{I_n(\beta_t)\}^{-1} U(\beta_t) && (4)
\end{aligned}$$

Fisher Scoring

$$\beta_{t+1} = \beta_t + \{I(\beta_t)\}^{-1} U(\beta_t)$$

Fisher scoring

Similar to Newton's method, but replace **observed information** for **Expected information**.

- Newton's method and Fisher scoring have the same asympotic properties, but for individual problems one or another may be easier computationally or analytically
    - I.E., for when observed information isn't semi positive definite and can't be inverted
- However, Newton's method and Fisher scoring are equivalent for GLM with canonical link
    - This is because the observed and expected information are the same in this setting (**check**!)

$$\beta_{t+1} = \beta_t + \{I(\beta_t)\}^{-1} U(\beta_t)$$

Iteratively reweighted least squares for GLM

In GLM, there is usually no closed form solution for the MLE, so the model fitting is done numerically as we've seen. In linear regression models, $E(y_i|x_i) = x_i^T\beta$, and we minimize

$$S(\beta) = \sum_i (y_i - x_i^T\beta)^2,$$

to get $\hat{\beta} = (X^TX)^{-1}X^TY$.

Question: For GLMs, can we minimize $S(\beta) = \sum_i (g(y_i) - x_i^T\beta)^2$? **Answer**: No, because $E(g(y|x)) \neq g(E(y|x)) = x^T\beta$, since g is nonlinear. This means we cannot transform y by g and then run linear regression.

Iteratively reweighted least squares

Idea: Approximate $g(y_i)$ by a linear function so that the OLS formula can be used.

Algorithm: at step t with current solution β^t, linearize $g(y_i)$ around $\hat{\mu}^t = g^{-1}(x_i^T \beta^t)$ (the fitted value for y_i at current step).

Denote the linearized value by $\tilde{y}_i^t$

$$\tilde{y}_i^t = g(\hat{\mu}^t) + (y_i - \hat{\mu}^t) g'(\hat{\mu}^t).$$

Now we can regress $\tilde{y}_i^t$ on x_i to estimate β^{t+1}. However, $\tilde{y}_i^t$ is heteroscedastic, i.e., the variances are not identical.

- For most distributions the variances is related to the mean.

Iteratively reweighted least squares

Derive the variances of $\tilde{y}_i^t$, and use the inverse of the variance as weights in a weighted least square (WLS):

$$W_i^t = [Var(\tilde{y}_i^t)]^{-1} = \left[\{g'(\hat{\mu}^t)\}^2 V(\hat{\mu}^t)\right]^{-1}$$

We can then minimize the following:

$$S(\beta) = \sum_i W_i^t (\tilde{y}_i^t - x_i^T \beta)^2.$$

Which gives solution

$$\hat{\beta} = (X^T W^t X)^{-1} (X^T W^t \tilde{y}^t)$$

Iterative reweighted least squares

IRLS algorithm:

1. Start with initial estimates, generally $\mu_i^0 = y_i$
2. Form $\tilde{y}^t$ and W^t
3. Estimate β^{t+1}
4. Form $\mu_i^{t+1} = g^{-1}(x_i^T \beta^{t+1})$, and return to step 2

- McCullagh and Nelder (1983) showed that IRLS is equivalent to Fisher scoring in **standard GLMs**.
- Using the canonical link, IRLS is also equivalent to Newton-Raphson

Inference on GLM parameter estimates

- $\hat{Var}(\hat{\theta}) = [I(\hat{\theta})]^{-1}$
- Then can use LRT, Wald, or Score test to obtain p-values and confidence intervals

Wald test statistic Z is given by

$$Z^2 = (\hat{\theta}_{MLE} - \theta_{H_0})^T [I(\hat{\theta}_{MLE})] (\hat{\theta}_{MLE} - \theta_{H_0}) \sim \chi^2_{df}$$

- **df** is the number of parameters being estimated in θ

Quasi-Newton

Quasi-Newton methods use Newton-like updates while avoiding repeated Hessian at each step.

- **Motivation**:
    - Computing H scales as $O(n^2)$, inverting it scales as $O(n^3)$
    - For 50-dimensional parameter, need to calculate $50(50+1)/2 = 1275$ values for H at each step, then perform another $\approx 50^3$ operations to invert it.

$$x_{t+1} = x_t - \{f''(x_t)\}^{-1} f'(x_t).$$

Quasi-Newton:

$$x_{t+1} = x_t - B_t^{-1} f'(x_t).$$

Where B_t is simpler to compute.

Quasi-Newton

Challenging because $f''(x_t)$ gives us a lot of information about the surface of f at x_t and throwing this out results in loss of information. Idea with Quasi-Newton is to find a solution B_t to the **secant equation**,

$$f'(x_t) - f'(x_{t-1}) = B_t(x_t - x_{t-1}).$$

In one dimension, this is simple. In multiple dimensions there are infinite solutions and we need to constrain the problem:

- B_t should be symmetric
- Should be close to B_{t-1}

Quasi-Newton

Let $y_t = f'(x_t) - f'(x_{t-1})$ and $s_t = x_t - x_{t-1}$ such that $y_t = B_t s_t$.

Broyden, Fletcher, Goldfarb, and Shanno (BFGS) update:

$$B_t = B_{t-1} + \frac{y_t y_t'}{y_t' s_t} - \frac{B_{t-1} s_t s_t' B_{t-1}'}{s_t' B_{t-1} s_t}$$

- Implemented in `optim()` function in R
- Initialize B_{t-1}^{-1}:
  - set $B_{t-1}^{-1} = I$
  - compute and invert true Hessian at initial point

Exercise

Add inference to your Newton's method for Poisson function.
Compare with results from glm().

Homework 3

Lab Exercise 3: Begin to implement Newton's method with inference for logistic regression (part 1 of Homework 3).

Resources

- Great blog post on Quasi Newton