Data Modeling and Least Squares Fitting 2

COS 323

Nonlinear Least Squares

- Some problems can be rewritten to linear

$$y = ae^{bx}$$

$$\Rightarrow \ (\log y) = (\log a) + bx$$

- Fit data points $(x_i, \log y_i)$ to $a^* + bx$, $a = e^{a^*}$
- Big problem: this no longer minimizes squared error!

Nonlinear Least Squares

- Can write error function, minimize directly

$$\chi^2 = \sum_i \left(y_i - f(x_i, a, b, \ldots)\right)^2$$

$$\text{Set } \frac{\partial}{\partial a} = 0, \frac{\partial}{\partial b} = 0, \text{ etc.}$$

- For the exponential, no analytic solution for a, b:

$$\chi^2 = \sum_i \left(y_i - ae^{bx_i}\right)^2$$

$$\frac{\partial}{\partial a} = \sum_i -2e^{bx_i}\left(y_i - ae^{bx_i}\right) = 0$$

$$\frac{\partial}{\partial b} = \sum_i -2ax_i e^{bx_i}\left(y_i - ae^{bx_i}\right) = 0$$

Newton's Method

- Apply Newton's method for minimization:

$$\begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i+1} = \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i} - H^{-1}G$$

where H is Hessian (matrix of all 2nd derivatives) and G is gradient (vector of all 1st derivatives)

Newton's Method for Least Squares

$$\chi^2 = \sum_i \left(y_i - f(x_i, a, b, \ldots)\right)^2$$

$$G = \begin{bmatrix} \frac{\partial(\chi^2)}{\partial a} \\ \frac{\partial(\chi^2)}{\partial b} \\ \vdots \end{bmatrix} = \begin{bmatrix} \sum_i -2\frac{\partial f}{\partial a}\left(y_i - f(x_i, a, b, \ldots)\right) \\ \sum_i -2\frac{\partial f}{\partial b}\left(y_i - f(x_i, a, b, \ldots)\right) \\ \vdots \end{bmatrix}$$

$$H = \begin{bmatrix} \frac{\partial^2(\chi^2)}{\partial a^2} & \frac{\partial^2(\chi^2)}{\partial a \partial b} & \cdots \\ \frac{\partial^2(\chi^2)}{\partial a \partial b} & \frac{\partial^2(\chi^2)}{\partial b^2} & \cdots \\ & \vdots & \end{bmatrix}$$

- Gradient has 1st derivatives of f, Hessian 2nd

Gauss-Newton Iteration

- Consider 1 term of Hessian:

$$\frac{\partial^2(\chi^2)}{\partial a^2} = \frac{\partial}{\partial a}\left(\sum_i -2\tfrac{\partial f}{\partial a}\big(y_i - f(x_i, a, b, \ldots)\big)\right)$$

$$= -2\sum_i \tfrac{\partial^2 f}{\partial a^2}\big(y_i - f(x_i, a, b, \ldots)\big) + 2\sum_i \tfrac{\partial f}{\partial a}\tfrac{\partial f}{\partial a}$$

- If close to answer, first term close to 0
- Gauss-Newton method: ignore first term!
  - Eliminates requirement to calculate 2nd derivatives of *f*

Gauss-Newton Iteration

$$\begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i+1} = \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i} + \delta_i$$

$$\mathrm{J}_i^{\mathrm{T}} \mathrm{J}_i \delta_i = \mathrm{J}_i^{\mathrm{T}} r_i$$

$$J = \begin{pmatrix} \frac{\partial f}{\partial a}(x_1) & \frac{\partial f}{\partial b}(x_1) & \cdots \\ \frac{\partial f}{\partial a}(x_2) & \frac{\partial f}{\partial b}(x_2) & \\ \vdots & & \ddots \end{pmatrix}, \quad r = \begin{pmatrix} y_1 - f(x_1, a, b, \cdots) \\ y_2 - f(x_2, a, b, \cdots) \\ \vdots \end{pmatrix}$$

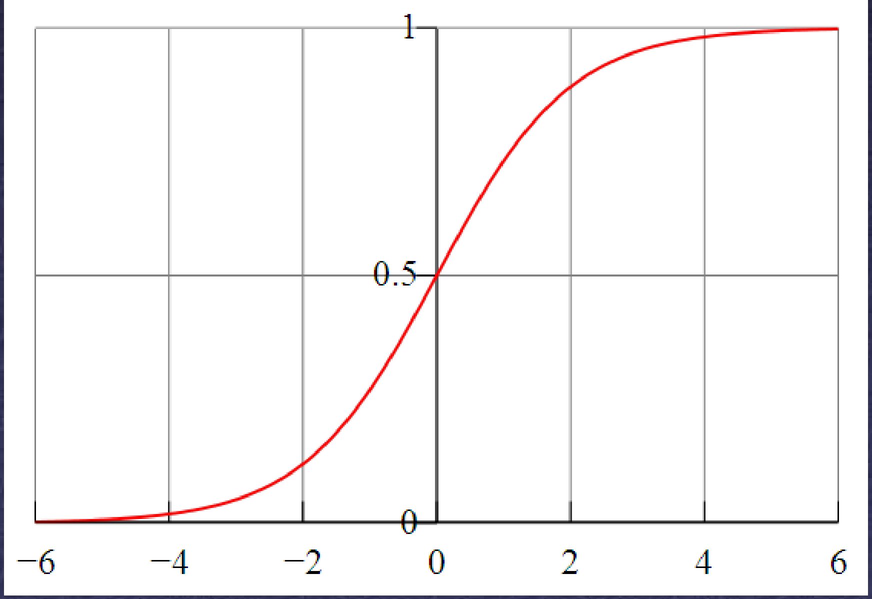
– Surprising fact: still superlinear convergence if “close enough” to answer

Example: Logistic Regression

- Model probability of an event based on values of explanatory variables, using generalized linear model, logistic function g(z)

$$p(\vec{x}) = g(ax_1 + bx_2 + \cdots)$$

$$g(z) = \frac{1}{1+e^{-z}}$$



Logistic Regression

- Uses assumption that positive and negative examples are normally distributed, with different means but same variance
- Applications: predict odds of election victories, sports events, medical outcomes, etc.
- Estimate parameters a, b, … using Gauss-Newton on individual positive, negative examples
- Handy hint: $g'(z) = g(z)\ (1-g(z))$

Levenberg-Marquardt

- Newton (and Gauss-Newton) work well when close to answer, terribly when far away
- Steepest descent safe when far away
- Levenberg-Marquardt idea: let's do both

$$\begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i+1} = \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i} - \alpha G - \beta \begin{pmatrix} \sum \frac{\partial f}{\partial a}\frac{\partial f}{\partial a} & \sum \frac{\partial f}{\partial a}\frac{\partial f}{\partial b} & \cdots \\ \sum \frac{\partial f}{\partial a}\frac{\partial f}{\partial b} & \sum \frac{\partial f}{\partial b}\frac{\partial f}{\partial b} & \cdots \\ & \vdots & \end{pmatrix}^{-1} G$$

Steepest descent

Gauss-Newton

Levenberg-Marquardt

- Trade off between constants depending on how far away you are…
- Clever way of doing this:

$$\begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i+1} = \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}_{i} - \begin{pmatrix} (1+\lambda)\Sigma \frac{\partial f}{\partial a}\frac{\partial f}{\partial a} & \Sigma \frac{\partial f}{\partial a}\frac{\partial f}{\partial b} & \cdots \\ \Sigma \frac{\partial f}{\partial a}\frac{\partial f}{\partial b} & (1+\lambda)\Sigma \frac{\partial f}{\partial b}\frac{\partial f}{\partial b} & \cdots \\ & \vdots & \end{pmatrix}^{-1} G$$

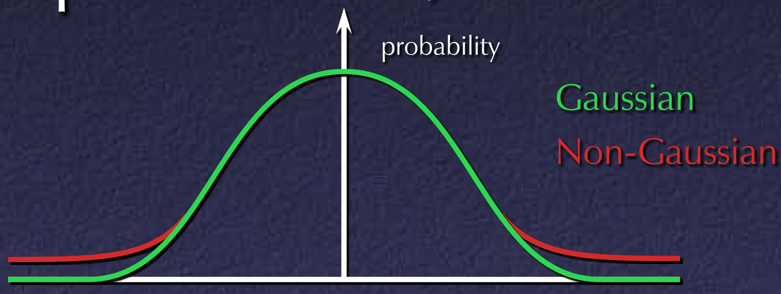
- If λ is small, mostly like Gauss-Newton
- If λ is big, matrix becomes mostly diagonal, behaves like steepest descent

Levenberg-Marquardt

- Final bit of cleverness: adjust λ depending on how well we're doing
  - Start with some λ, e.g. 0.001
  - If last iteration *decreased* error, *accept* the step and *decrease* λ to $\lambda/10$
  - If last iteration *increased* error, *reject* the step and *increase* λ to 10λ
- Result: fairly stable algorithm, not too painful (no 2nd derivatives), used a lot

Outliers

- A lot of derivations assume Gaussian distribution for errors
- Unfortunately, nature (and experimenters) sometimes don't cooperate



- Outliers: points with extremely low probability of occurrence (according to Gaussian statistics)
- Can have strong influence on least squares

Robust Estimation

- Goal: develop parameter estimation methods insensitive to *small* numbers of *large* errors
- General approach: try to give large deviations less weight
- M-estimators: minimize some function other than square of $y - f(x,a,b,\ldots)$

Least Absolute Value Fitting

- Minimize $\sum_i \left| y_i - f(x_i, a, b, \ldots) \right|$
  instead of $\sum_i \left(y_i - f(x_i, a, b, \ldots) \right)^2$

- Points far away from trend get comparatively less influence

Example: Constant

- For constant function $y = a$, minimizing $\Sigma(y-a)^2$ gave $a = \text{mean}$
- Minimizing $\Sigma|y-a|$ gives $a = \text{median}$

Doing Robust Fitting

- In general case, nasty function: discontinuous derivative
- Simplex method often a good choice

Iteratively Reweighted Least Squares

- Sometimes-used approximation:
  convert to iterated weighted least squares

$$
\begin{aligned}
&\sum_i \left| y_i - f(x_i, a, b, \ldots) \right| \\
&= \sum_i \frac{1}{\left| y_i - f(x_i, a, b, \ldots) \right|} \big(y_i - f(x_i, a, b, \ldots) \big)^2 \\
&= \sum_i w_i \big(y_i - f(x_i, a, b, \ldots) \big)^2
\end{aligned}
$$

with w_i based on previous iteration

M-Estimators

Different options for weights

- Avoid problems with infinities
- Give even less weight to outliers

$$w_i = \frac{1}{\left|y_i - f(x_i, a, b, \ldots)\right|}$$ L$_1$

$$w_i = \frac{1}{\varepsilon + \left|y_i - f(x_i, a, b, \ldots)\right|}$$ "Fair"

$$w_i = \frac{1}{\varepsilon + \left(y_i - f(x_i, a, b, \ldots)\right)^2}$$ Cauchy / Lorentzian

$$w_i = e^{-k\left(y_i - f(x_i, a, b, \ldots)\right)^2}$$ Welsch

Iterratively Reweighted Least Squares

- Danger! This is not guaranteed to converge to the right answer!
  - Needs good starting point, which is available if initial least squares estimator is reasonable
  - In general, works OK if few outliers, not too far off

Outlier Detection and Rejection

- Special case of IRWLS: set weight = 0 if outlier, 1 otherwise
- Detecting outliers: $(y_i - f(x_i))^2 >$ threshold
  - One choice: multiple of mean squared difference
  - Better choice: multiple of *median* squared difference
  - Can iterate…
  - As before, not guaranteed to do anything reasonable, tends to work OK if only a few outliers

RANSAC

- RANdom SAmple Consensus: desgined for bad data (in best case, up to 50% outliers)
- Take many random subsets of data
  - Compute least squares fit for each sample
  - See how many points agree: $(y_i - f(x_i))^2 <$ threshold
  - Threshold user-specified or estimated from more trials
- At end, use fit that agreed with most points
  - Can do one final least squares with all inliers