Logistic Regression: Behind the Scenes

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Capital One

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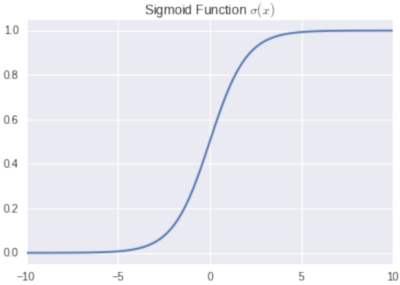
Generative Model

$$y_i|\beta, x_i \sim \text{Bernoulli}\big(\sigma(\beta, x_i)\big)$$

where

$$\sigma(\beta, x) := \frac{1}{1 + \exp\left(-\beta \cdot x\right)}$$

is the *sigmoid* function.



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Question: Given data, how do we determine the "best" values for β?

Typical Answer

Maximum Likelihood Estimation

$$\beta^* = \arg\max_{\beta} \prod_i \sigma\left(\beta \cdot x_i\right)^{y_i} \left(1 - \sigma\left(\beta \cdot x_i\right)\right)^{1-y_i}$$

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- **Note:** *the likelihood is a function of the predicted probabilities and the observed response*

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The story doesn't end here!

Uncritically throwing your data into an off-the-shelf solver could result in a bad model.

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Goal

We want to explore these questions with an eye on statsmodels, scikit-learn and SAS's proc logistic.

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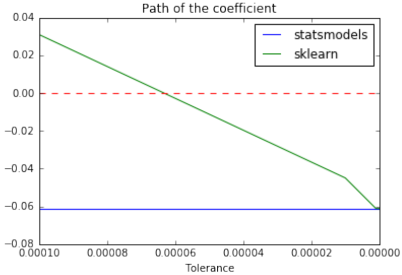

Prediction vs. Inference, cont'd

Coefficients and Multicollinearity

- Linear models are invariant under affine transformations of the data; this leads to a determination problem in the presence of "high" multicollinearity
- Multicollinearity can threaten long term model stability
- Can test for multicollinearity with condition number or Variance Inflation Factors (VIF)

Default Convergence Criteria

Tool	Algorithm	Convergence	Default Tol
SAS proc logistic	IRWLS	Relative Gradient	10^{-8}
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Note

Convergence criteria based on log-likelihood convergence emphasize *prediction stability*.

Behavior under different implementations

Especially in edge cases (e.g. quasi-separability, high multicollinearity) slightly different implementations can lead to drastically different outputs.

At github.com/moody-marlin/pydata_logistic you can find a notebook with various implementations of Newton's method for logistic regression, with explanations.

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Scoring conventions

- scikit-learn and ‘base’ statsmodels will score by *location*
- SAS and statsmodels + formula can score by name

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...and if not, can you compute it? For example, sklearn *always* uses regularization, computing p-values yourself will be incorrect!

Rant on *p*-values

Imagine a misspecified ordinary least squares model in which the true specification takes the form $y \sim \mathcal{N}(f(x), \sigma^2)$ for some *non-linear* $f(x)$.

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The MLE is given by

$$\beta^* = x^T y \|x\|_2^{-2}$$

and converges to its expectation in the limit $n \to \infty$, i.e.,

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Conclusion

Note that $\lim_{n\to\infty} \beta^* > 0$ if and only if $\mathbb{E}_x \left[x^T \vec{f}(x) \right] > 0$.

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Takeaway

p-values and Big Data are not friends!

Regularization

Regularization is the process of "penalizing" candidate coefficients for undesirable complexity, i.e.,

$$\beta^* = \arg\max_{\beta} \mathcal{L}\left(x, y, \beta\right) - \tau g(\beta)$$

where $g(\beta)$ is some application-dependent measure of "complexity", and $\tau > 0$.

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Be aware

Regularization means your estimated coefficients are *no longer* maximum likelihood estimators, so be careful in your interpretation and inference!

Caution!

Many optimization options subtly result in regularization!

- the ‘FIRTH’ option in SAS (and ‘logistf’ in R) arise from setting $g(\beta) = \log\left(\det \mathcal{I}(\beta)\right)$ and $\tau = \frac{1}{2}$, where $\mathcal{I}(\beta)$ is the Fisher information matrix

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- sklearn *always* regularizes

Statistical Implications: Bayesian Interpretation

Any regularization function for which

$$\int_{\mathbb{R}^k} \exp\left(-g(\beta)\right) d\beta < \infty$$

results in a penalized log-likelihood with a Bayesian interpretation.

The regularized coefficients are maximum a posteriori (MAP) estimators for a Bayesian model with prior distribution given by

$$\exp\left(-g(\beta)\right)$$

.

Conclusion

Takeaway

Even if you don't run into any edge cases, understanding what's happening under the hood gives you access to *much more* information that you can leverage to build better, more informative models!

The End

Thanks for your time and attention! Questions?