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Python中优化方法

`statsmodels.discrete.discrete_model.Logit.fit(start_params=None, method='newton', maxiter=35, full_output=1, disp=1, callback=None, **kwargs)`

method可选择的有：

- 'newton': Newton-Raphson
- 'nm': Nelder-Mead Simplex algorithm
- 'bfgs': Broyden-Fletcher-Goldfarb-Shanno algorithm
- 'lbfgs': limited-memory BFGS with optional box constraints
- 'powell': modified Powell's method
- 'cg': conjugate gradient
- 'ncg': Newton-Conjugate-Gradient algorithm
- 'basinhopping': global basin-hopping solver
- 'minimize': generic wrapper of scipy minimize (BFGS by default)

`sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None)`

`solver{'newton-cg', 'lbfgs', 'liblinear', 'sag', 'saga'}, default='lbfgs'`

- For small datasets, 'liblinear' is a good choice, whereas 'sag' and 'saga' are faster for large ones.

- For multiclass problems, only ‘newton-cg’, ‘sag’, ‘saga’ and ‘lbfgs’ handle multinomial loss; ‘liblinear’ is limited to one-versus-rest schemes.
- ‘newton-cg’, ‘lbfgs’, ‘sag’ and ‘saga’ handle L2 or no penalty
- ‘liblinear’ and ‘saga’ also handle L1 penalty
- ‘saga’ also supports ‘elasticnet’ penalty
- ‘liblinear’ does not support setting `penalty='none'`

Note that ‘sag’ and ‘saga’ fast convergence is only guaranteed on features with approximately the same scale. You can preprocess the data with a scaler from `sklearn.preprocessing`.

New in version 0.17: Stochastic Average Gradient descent solver.

New in version 0.19: SAGA solver.

优化方法

符号说明：

- $g_k = g(x^{(k)}) = \nabla f(x^{(k)})$ 为 $f(x)$ 在 $x^{(k)}$ 处的梯度
- λ_k 为步长, $\lambda_k \geq 0$
- $H_k = H(x^{(k)}) = [\frac{\partial^2 f}{\partial x_i^{(k)} \partial x_j^{(k)}}]_{n \times n}$ 为 Hessian 矩阵
- G_k 近似 H_k^{-1} , B_k 近似 H_k
- $y_k = g_{k+1} - g_k$, $\delta_k = x^{(k+1)} - x^{(k)}$
- 牛顿条件: $\delta_k = H_k^{-1} y_k$ 或 $y_k = H_k \delta_k$
-

不同算法：

- 梯度下降 gradient descent (又称“最速下降法 steepest descent”)

$$\min_x f(x) \quad f(x) \text{一阶可导} \quad (1)$$

$$f(x) = f(x^{(k)}) + g_k^T (x - x^{(k)}) \quad (2)$$

$$\Rightarrow x^{(k+1)} = x^{(k)} - \lambda_k g_k \quad (3)$$

- Newton method

$$\min_x f(x) \quad f(x) \text{二阶可导} \quad (4)$$

$$f(x) = f(x^{(k)}) + g_k^T(x - x^{(k)}) + \frac{1}{2}(x - x^{(k)})^T H_k(x - x^{(k)}) \quad (5)$$

$$\Rightarrow \nabla f(x) = g_k + H_k(x - x^{(k)}) \quad (6)$$

$$\Rightarrow x^{(k+1)} = x^{(k)} - H_k^{-1} g_k \quad (7)$$

$$g_{k+1} - g_k = H_k(x^{(k+1)} - x^{(k)}) \Rightarrow y_k = H_k \delta_k$$

quasi-Newton method将Newton method中的 H_k^{-1} 用其他矩阵来逼近

- quasi-Newton method: DFP algorithm (Davidon-Fletcher-Powell)

$$G_{k+1} = G_k + P_k + Q_k \quad (8)$$

$$G_{k+1} y_k = G_k y_k + P_k y_k + Q_k y_k \quad (9)$$

$$\text{令 } P_k y_k = \delta_k, Q_k y_k = -G_k y_k \quad (10)$$

$$\Rightarrow P_k = \frac{\delta_k \delta_k^T}{\delta_k^T y_k}, Q_k = -\frac{G_k y_k y_k^T G_k}{y_k^T G_k y_k} \quad (11)$$

$$\Rightarrow G_{k+1} = G_k + \frac{\delta_k \delta_k^T}{\delta_k^T y_k} - \frac{G_k y_k y_k^T G_k}{y_k^T G_k y_k} \quad (12)$$

$$\Rightarrow x^{(k+1)} = x^{(k)} - \lambda_k G_k g_k \quad (13)$$

初始 G_0 须设定为正定矩阵, 则迭代过程中的每个 G_k 都是正定的.

- quasi-Newton method: BFGS algorithm (Broyden-Fletcher-Goldfarb-Shannon)

$$B_{k+1} = B_k + P_k + Q_k \quad (14)$$

$$B_{k+1} \delta_k = B_k \delta_k + P_k \delta_k + Q_k \delta_k \quad (15)$$

$$\text{令 } P_k \delta_k = y_k, Q_k \delta_k = -B_k \delta_k \quad (16)$$

$$\Rightarrow B_{k+1} = B_k + \frac{y_k y_k^T}{y_k^T \delta_k} - \frac{B_k \delta_k \delta_k^T B_k}{\delta_k^T \delta_k} \quad (17)$$

$$G_k = B_k^{-1} \Rightarrow G_{k+1} = (I - \frac{\delta_k y_k^T}{\delta_k^T y_k}) G_k (I - \frac{\delta_k y_k^T}{\delta_k^T y_k})^T + \frac{\delta_k \delta_k^T}{\delta_k^T y_k} \quad (18)$$

$$\Rightarrow x^{(k+1)} = x^{(k)} - \lambda_k B_k^{-1} g_k, \quad x^{(k+1)} = x^{(k)} - \lambda_k G_k g_k \quad (19)$$

初始 G_0 须设定为正定矩阵, 则迭代过程中的每个 G_k 都是正定的.

- quasi-Newton method: Broyden's algorithm

$$G_{k+1} = \alpha G^{DFP} + (1 - \alpha) G^{BFGS}, 0 \leq \alpha \leq 1$$

其中 G^{DFP} 表示DFP算法计算出的 G ， G^{BFGS} 表示BFGS算法计算出的 G 。

坐标轴下降法 求解Lasso回归

coordinate descent: 一个可微的凸函数 $J(\theta)$ ，其中 θ 是 $n \times 1$ 的向量，即有 n 个维度。若在某一点 $\bar{\theta}_i (i = 1, 2, \dots, n)$ 上都是最小值，则 $J(\bar{\theta}_i)$ 就是一个全局的最小值。

1. 初始化 $\theta^{(0)}$
2. 从 $\theta_1^{(k)}$ 到 $\theta_n^{(k)}$ ，依次求 $\theta_i^{(k)}$ ， $\theta_i^{(k)} = \arg \min_{\theta_i} J(\theta_1^{(k)}, \theta_2^{(k)}, \dots, \theta_{i-1}^{(k)}, \theta_i, \theta_{i+1}^{(k-1)}, \dots, \theta_n^{(k-1)})$
3. 迭代至在所有维度上变化都比较小

最小角回归法 求解Lasso回归

Logistic回归

1. 指数族分布角度的Logistic回归

(1)指数族分布

指数族分布 $f(y; \theta, \phi) = \exp\{\frac{y\theta - b(\theta)}{a(\phi)} + c(y, \phi)\}$ ，其中 θ 为自然参数， ϕ 为散度参数， a, b, c 为函数，且满足以下条件：

- $a(\phi) > 0$ ，连续，通常为 ϕ/w ，其中 w 为已知先验权重
- $b(\theta)$ 二阶导数存在且大于零
- $c(y, \phi)$ 与参数 θ 无关

指数族分布的性质如下：

$$E(Y) = b'(\theta) \quad (20)$$

$$Var(Y) = b''(\theta)a(\phi) = V(\mu)a(\phi), \text{其中} V(\mu) = b''(\theta) \text{为指数族分布的方差函数.} \quad (21)$$

$$\mu = E(Y) \quad (22)$$

$$\eta = X^T \beta \quad (23)$$

线性预测量 $\eta = X^T\beta$ 和 Y 的期望之间，通过一个单调的连接函数 $g(\cdot)$ 联系在一起，即 $g(\mu) = \eta$:

- $g(\mu) = \ln\mu \quad (\mu > 0)$
- $g(\mu) = \ln\frac{\mu}{1-\mu} \quad 0 < \mu < 1$
- $g(\mu) = \Phi^{-1}(\mu) \quad 0 < \mu < 1$
- ...

Logistic的LinkFunction为 $g(\mu) = \ln\frac{\mu}{1-\mu} \quad 0 < \mu < 1$, $g(\mu_i) = \sum_{j=1}^p X_{ij}\beta_j, \quad i = 1, \dots, n$

(2)Logistic回归

设 X_1, \dots, X_p 的 n 组值 $X_i = (X_{i1}, \dots, X_{ip})^T, i = 1, \dots, n$ 在每个 X_i 处，对二值随机变量 ξ_i 进行 m_i 次观测，其中 $\xi_i = 1$ 表示发生事件A， $\xi_i = 0$ 表示未发生事件A.

设 $\xi_i = 1$ 有 k_i 次，令 Y_i 表示 $\{\xi_i = 1\}$ 出现的频率，则 $Y_i = \frac{k_i}{m_i}, i = 1, \dots, n, k_i = 0, 1, 2, \dots, m_i$.

设 Y_1, \dots, Y_n 相互独立，则 $Y_i \sim B(m_i, \mu_i)/m_i, i = 1, \dots, n$, 即 $X_i = Y_i m_i \sim B(m_i, \mu_i)$.

$$P(Y = y) = P(X = ym) = C_m^{my} \mu^{my} (1 - \mu)^{m-my} = \exp\left\{\frac{y \ln \frac{\mu}{1-\mu} + \ln(1-\mu)}{1/m} + \ln(C_m^{my})\right\}.$$

$$\Rightarrow \theta = \ln \frac{\mu}{1-\mu}, \phi = \frac{1}{m}, a(\phi) = \phi = \frac{1}{m}, b(\theta) = -\ln(1 - \mu) = \ln(1 + e^\theta), c(y, \phi) = \ln C_m^{my}.$$

设 $Y_i \sim f(y; \theta_i, \phi_i) = \exp\left\{\frac{y\theta_i - b(\theta_i)}{a(\phi_i)} + c(y, \phi_i)\right\}$ ，则其对数似然函数为

$$\ln L(\beta_1, \dots, \beta_p) = \ln \left[\sum_{i=1}^n f(Y_i; \theta_i, \phi_i) \right] = \sum_{i=1}^n \left[\frac{Y_i \theta_i - b(\theta_i)}{a(\phi_i)} + c(Y_i, \phi_i) \right] \quad (24)$$

$$\Rightarrow \frac{\partial \ln L(\beta_1, \dots, \beta_p)}{\partial \beta_r} = \frac{\partial \sum_{i=1}^n \frac{Y_i \theta_i - b(\theta_i)}{a(\phi_i)}}{\partial \beta_r} = 0, \quad r = 1, \dots, p \quad (25)$$

$$\Rightarrow \sum_{i=1}^n \frac{(Y_i - \mu_i) X_{ir}}{a(\phi_i) V(\mu_i) g'(\mu_i)} = 0, \quad \mu_i = g^{-1} \left(\sum_{j=1}^p X_{ij} \beta_j \right), \quad r = 1, \dots, p \quad (26)$$

(3)求解方法

$$\sum_{i=1}^n \frac{(Y_i - \mu_i) X_{ir}}{a(\phi_i) V(\mu_i) g'(\mu_i)} = 0, \quad \mu_i = g^{-1} \left(\sum_{j=1}^p X_{ij} \beta_j \right), \quad r = 1, \dots, p$$

需通过迭代法来求解 β

IRWLS

设 $Y_i \sim N(\mu_i, \sigma_i^2)$, $\sigma_i^2 = \sigma^2 a_i$ 且 $a_1 \dots a_n$ 已知, Y_i 与 X_1, \dots, X_p 服从线性模型, 则

$$\mu_i = E(Y_i) = g(\mu_i) = \sum_{j=1}^p X_{ij} \beta_j \quad (27)$$

$$g(\mu) = \mu, V(\mu) = b''(\theta) = 1, a(\phi) = a_i \phi = a_i \sigma^2 = \sigma_i^2, b(\theta) = \frac{\theta^2}{2}, \theta = \mu \quad (28)$$

$$\Rightarrow \sum_{i=1}^n \frac{(Y_i - \mu_i) X_{ir}}{a(\phi_i) V(\mu_i) g'(\mu_i)} = \sum_{i=1}^n \frac{Y_i - \mu_i}{a_i} X_{ir} = 0 \quad (29)$$

$$Y = (y_1, y_2, \dots, y_n)^T, X = \begin{bmatrix} X_{11} & X_{12} & \dots & X_{1p} \\ X_{21} & X_{22} & \dots & X_{2p} \\ \dots & \dots & \dots & \dots \\ X_{n1} & X_{n2} & \dots & X_{np} \end{bmatrix}_{n \times p}, \quad (30)$$

$$\beta = (\beta_1, \dots, \beta_p)^T, W = \text{Diag}(\frac{1}{a_1}, \dots, \frac{1}{a_n}) \quad (31)$$

$$\Rightarrow \hat{\beta} = (X^T W X)^{-1} X^T W Y \quad (32)$$

令 $Z_i = g(\mu_i) + (Y_i - \mu_i) g'(\mu_i)$, 则 $E(Z_i) = g(\mu_i)$, $\text{Var}(Z_i) = a_i \phi V(\mu_i) [g'(\mu_i)]^2 = \tilde{a}_i \phi$.

\Rightarrow 线性模型 $E(Z_i) = \sum_{j=1}^p X_{ij} \beta_j$ 的似然方程为 $\sum_{i=1}^n \frac{Z_i - g(\mu_i)}{\tilde{a}_i} X_{ir} = \sum_{i=1}^n \frac{Y_i - \mu_i}{a_i V(\mu_i)} \frac{X_{ir}}{g'(\mu_i)} = 0$.

$$\Rightarrow \hat{\beta} = (X^T W X)^{-1} X^T W Z$$

$$\eta_i^{(t)} = g(\mu_i^{(t)}) = \sum_{j=1}^p X_{ij} \beta_j^{(t)} \quad (33)$$

$$Z_i^{(t)} = \eta_i^{(t)} + (Y_i - \mu_i^{(t)}) g'(\mu_i^{(t)}) \quad (34)$$

$$W_i^{(t)} = \frac{1}{a_i V(\mu_i^{(t)}) [g'(\mu_i^{(t)})]^2} \quad (35)$$

$$\hat{\beta}^{(t+1)} = (X^T W^{(t)} X)^{-1} X^T W^{(t)} Z^{(t)} \quad (36)$$

IRWLS迭代步骤:

1. 给定一组初值 $\mu_1^{(0)}, \dots, \mu_n^{(0)}$, 如 $\mu_i^{(0)} = Y_i$
2. 计算 $\eta_i^{(0)} = g(\mu_i^{(0)})$, Logistic中连接函数 $g(\mu) = \ln \frac{\mu}{1-\mu} \quad 0 < \mu < 1$
3. 计算 $Z_i^{(0)} = \eta_i^{(0)} + (Y_i - \mu_i^{(0)}) g'(\mu_i^{(0)})$
4. 计算 $W_i^{(0)} = \frac{1}{a_i V(\mu_i^{(0)}) [g'(\mu_i^{(0)})]^2}$

5. 求出 $\hat{\beta}^{(1)} = (X^T W^{(0)} X)^{-1} X^T W^{(0)} Z^{(0)}$, 其中 $Z^{(0)} = (Z_1^{(0)}, Z_2^{(0)}, \dots, Z_n^{(0)})^T$, $W^{(0)} = \text{Diag}(W_1^{(0)}, W_2^{(0)}, \dots, W_n^{(0)})$
6. 令 $\eta^{(1)} = (\eta_1^{(1)}, \eta_2^{(1)}, \dots, \eta_n^{(1)})^T = X \hat{\beta}^{(1)}$, 进而求出 $Z_i^{(1)}, W_i^{(1)}, \hat{\beta}^{(1)}$
7. 迭代至 $\hat{\beta}^{(t+1)}$ 收敛

在Logistic回归中, $g(\mu) = \ln \frac{\mu}{1-\mu}$ $0 < \mu < 1$, $g'(\mu) = \frac{1}{\mu(1-\mu)}$, $V(\mu) = b''(\theta) = \mu(1-\mu)$, 代入IRWLS迭代步骤, 即可求出Logistic模型中的估计系数 $\hat{\beta}$ 。

Newton-Raphson迭代法与Fisher得分法

对数似然函数 $f(\beta) = \ln L(\beta_1, \dots, \beta_p) = \sum_{i=1}^n [\frac{Y_i \theta_i - b(\theta_i)}{a(\phi_i)} + c(Y_i, \phi_i)]$

$$\mu_i = b'(\theta_i), g(\mu_i) = \sum_{j=1}^p X_{ij} \beta_j$$

求解 $\hat{\beta} = \arg \max_{\beta} f(\beta)$

Newton-Raphson迭代法:

- 设 $f(\beta)$ 是 $\beta = (\beta_1, \dots, \beta_p)^T$ 的 p 元函数, 求 $\hat{\beta}$ 使 $f(\hat{\beta}) = \max_{\beta} f(\beta)$
- 令 $q = (q_1, \dots, q_p)^T = (\frac{\partial f(\beta)}{\partial \beta_1}, \dots, \frac{\partial f(\beta)}{\partial \beta_p})^T = \frac{\partial f(\beta)}{\partial \beta}$, $H = (h_{kl})_{p \times p} = \frac{\partial^2 f(\beta)}{\partial \beta \partial \beta^T}$, $h_{kl} = \frac{\partial^2 f(\beta)}{\partial \beta_l \partial \beta_k}$, $0 \leq k, l \leq p$
- $q^{(t)} = \frac{\partial f(\beta)}{\partial \beta} |_{\beta=\beta^{(t)}}$, $H^{(t)} = (h_{kl}^{(t)})$, $h_{kl}^{(t)} = \frac{\partial^2 f(\beta)}{\partial \beta_l \partial \beta_k} |_{\beta=\hat{\beta}^{(t)}}$
- $f(\beta)$ 在 $\beta = \hat{\beta}^{(t)}$ 处的二次Taylor展开: $f(\beta) \approx Q^{(t)}(\beta) = f(\beta^{(t)}) + (q^{(t)})^T (\beta - \beta^{(t)}) + \frac{1}{2} (\beta - \beta^{(t)})^T H^{(t)} (\beta - \beta^{(t)})$
- 令 $\frac{\partial Q^{(t)}(\beta)}{\partial \beta} = q^{(t)} + H^{(t)} (\beta - \beta^{(t)}) = 0$, $\Rightarrow \hat{\beta}^{(t+1)} = \beta^{(t)} - [H^{(t)}]^{-1} q^{(t)}$, $t = 0, 1, 2, \dots$

求多元函数极值问题的Newton-Raphson公式为

$$\hat{\beta}^{(t+1)} = \beta^{(t)} - [H^{(t)}]^{-1} q^{(t)}, \quad t = 0, 1, 2, \dots \quad (\text{N-R})$$

设指数族分布中的 $a(\phi_i) = a_i \phi$ 且 $a_i \dots a_n$ 已知

- 得分向量Score Vector: $f(\beta)$ 关于 β_1, \dots, β_p 的一阶偏导数所成的向量

$$\frac{\partial f(\beta)}{\partial \beta_k} = \frac{\partial \ln L(\beta_1, \dots, \beta_p)}{\partial \beta_k} = \sum_{i=1}^n \frac{Y_i - \mu_i}{a_i \phi V(\mu_i) g'(\mu_i)} X_{ik}, \quad k = 1, \dots, p \quad (37)$$

$$\mu_i = g^{-1}\left(\sum_{j=1}^p X_{ij} \beta_j\right), \quad i = 1, \dots, n \quad (38)$$

$$\text{Score Vector: } S(\beta; Y) = (S_1(\beta; Y), \dots, S_p(\beta; Y))^T = \left(\frac{\partial f(\beta)}{\partial \beta_1}, \dots, \frac{\partial f(\beta)}{\partial \beta_p}\right)^T \quad (39)$$

- 信息阵 I : 是Newton_Raphson迭代中的Hessian矩阵 H 的负矩阵

$$\text{信息阵各元素 } I_{kl}(\beta; Y) = -\frac{\partial^2 f(\beta)}{\partial \beta_l \partial \beta_k} = -\frac{\partial}{\partial \beta_l} \left(\frac{\partial f(\beta)}{\partial \beta_k} \right) = -\frac{\partial}{\partial \beta_l} \left(\sum_{i=1}^n \frac{Y_i - \mu_i}{a_i \phi V(\mu_i) g'(\mu_i)} X_{ik} \right) \quad (40)$$

$$= -\sum_{i=1}^n \left[\frac{Y_i - \mu_i}{a_i \phi} \frac{\partial}{\partial \beta_l} \left(\frac{X_{ik}}{V(\mu_i) g'(\mu_i)} \right) - \frac{X_{ik} X_{il}}{a_i \phi V(\mu_i) [g'(\mu_i)]^2} \right] \quad (41)$$

$$I(\beta; Y) = (I_{kl}(\beta; Y))_{p \times p} = -H \quad (42)$$

- Fisher信息阵: 是信息阵 I 的期望

$$\text{Fisher Information Matrix: } F(\beta) = E(I(\beta; Y)) = E(I_{kl}(\beta; Y)) = -E(H) \quad (43)$$

$$\Rightarrow E(I_{kl}(\beta; Y)) = \sum_{i=1}^n \frac{X_{ik} X_{il}}{a_i \phi V(\mu_i) (g'(\mu_i))^2} = \frac{1}{\phi} \sum_{i=1}^n W_i X_{ik} X_{il}, \quad W_i = \frac{1}{a_i V(\mu_i) (g'(\mu_i))^2} \quad (44)$$

$$\Rightarrow E(I_{kl}(\beta; Y)) = \frac{1}{\phi} (X^T W X)_{kl}, \quad W = \text{Diag}(W_1, \dots, W_n), \quad \text{与IRWLS中的} W \text{相同} \quad (45)$$

$$\Rightarrow F(\beta) = \frac{1}{\phi} (X^T W X)_{kl}, \quad F^{-1}(\beta) = \phi (X^T W X)^{-1} \quad (46)$$

- GLM中的Newton-Raphson迭代法

$$\hat{\beta}^{(t+1)} = \hat{\beta}^{(t)} + I^{-1}(\hat{\beta}^{(t)}; Y) S(\hat{\beta}^{(t)}; Y), \quad t = 0, 1, 2, \dots$$

I^{-1} 中有因子 ϕ , S 中有因子 $\frac{1}{\phi}$, 故迭代公式与未知量 ϕ 无关.

- Fisher得分法(又称为“修正的N-R法”): 用“Fisher信息阵 F ”代替“信息阵 I ”

$$\hat{\beta}^{(t+1)} = \hat{\beta}^{(t)} + F^{-1}(\hat{\beta}^{(t)}; Y) S(\hat{\beta}^{(t)}; Y), \quad t = 0, 1, 2, \dots$$

可证明Fisher得分法与IRWLS法等价

将Logistic模型中

$$\theta = g(\mu) = \ln \frac{\mu}{1-\mu} = X^T \beta \quad (47)$$

$$\phi = \frac{1}{m}, a(\phi) = \phi = \frac{1}{m} \quad (48)$$

$$b(\theta) = -\ln(1-\mu) = \ln(1+e^\theta) \quad (49)$$

$$c(y, \phi) = \ln C_m^{my} \quad (50)$$

$$V(\theta) = b''(\theta) = \frac{e^\theta}{(1+e^\theta)^2} = \mu(1-\mu) \quad (51)$$

代入上述IRWLS、Newton-Raphson、Fisher得分法的迭代公式中，即可求出 $\hat{\beta}$ 。

2. 直接定义Logistic模型

$$P(Y = 1|X = x_i) = \frac{\exp(\beta_0 + x_i^T \beta)}{1 + \exp(\beta_0 + x_i^T \beta)} = p_i \quad (52)$$

$$P(Y = 0|X = x_i) = \frac{1}{1 + \exp(\beta_0 + x_i^T \beta)} = 1 - p_i \quad (53)$$

$$\text{logit}(p) = \ln \frac{p}{1-p} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p \quad (54)$$

$$\theta = (\beta_0, \beta^T)^T \quad (55)$$

$$L(\theta) = \ln \prod_{i=1}^n [p(x_i)]^{y_i} [1 - p(x_i)]^{1-y_i} \quad (56)$$

$$= \sum_{i=1}^n [y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i)] \quad (57)$$

$$= \sum_{i=1}^n [y_i \ln\left(\frac{p_i}{1 - p_i}\right) + \ln(1 - p_i)] \quad (58)$$

$$= \sum_{i=1}^n [y_i (\beta_0 + x_i^T \beta) + \ln(1 - \frac{e^{\beta_0 + x_i^T \beta}}{1 + e^{\beta_0 + x_i^T \beta}})] \quad (59)$$

$$= \sum_{i=1}^n [y_i (\beta_0 + x_i^T \beta) - \ln(1 + e^{\beta_0 + x_i^T \beta})] \quad (60)$$

$$\Rightarrow \begin{cases} \frac{\partial \ln[L(\theta)]}{\partial \beta_0} = \sum_{i=1}^n [y_i - \frac{e^{\beta_0 + x_i^T \beta}}{1 + e^{\beta_0 + x_i^T \beta}}] \\ \frac{\partial \ln[L(\theta)]}{\partial \beta} = \sum_{i=1}^n [y_i - \frac{e^{\beta_0 + x_i^T \beta}}{1 + e^{\beta_0 + x_i^T \beta}}] x_i \end{cases} \quad (61)$$

参考资料

- [1] <https://liushulun.cn/post/machinelearning/ml-logistic/data-ml-logistic-optimization/ml-logistic-optimization/>
- [2] <https://blog.csdn.net/lipengcn/article/details/52698895> (LBFGS)
- [3] <https://liuxiaofei.com.cn/blog/lbfgs方法推导/#lbfgs方法推导> (LBFGS)
- [4] <https://www.cnblogs.com/pinard/p/6018889.html> (坐标轴下降法与最小角回归法)
- [5] <https://www.cs.cmu.edu/~ggordon/10725-F12/slides/> (PPT优化方法)