Logistic Regression and Convex Optimization

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Logistic Regression

Binary:
$$P(Y = 1 | X = x) = \frac{1}{1 + e^{w^{\top}x}}$$

Multiclass:
$$P(Y = y_k \mid X = \boldsymbol{x}) = \frac{e^{\boldsymbol{w}_k^\top \boldsymbol{x}}}{1 + \sum_{k'=1}^{K-1} e^{\boldsymbol{w}_{k'}^\top \boldsymbol{x}}}$$

Logistic Regression Decision Boundary

Linear classification boundary, but why?

$$P(Y = 1 | X = x) = P(Y = 0 | X = x) \Rightarrow$$

$$\frac{1}{1 + e^{w^{\top}x}} = \frac{e^{w^{\top}x}}{1 + e^{w^{\top}x}} \Rightarrow$$

$$w^{\top}x = 0$$

$$Multiclass: Voronoi$$
Hyperplane

Training Logistic Regression

We use maximum condition likelihood estimation (MCLE):

$$\boldsymbol{w} = \arg \max_{\boldsymbol{w}} \prod_{i=1}^{n} P(Y = y^{i} \mid X = \boldsymbol{x}^{i}, \boldsymbol{w}) \Rightarrow$$
$$\boldsymbol{w} = \arg \max_{\boldsymbol{w}} \sum_{i=1}^{n} y^{i}(\boldsymbol{w}^{\top}\boldsymbol{x}^{i}) - \log(1 + e^{\boldsymbol{w}^{\top}\boldsymbol{x}^{i}})$$

But how do we solve this?

Convex Optimization

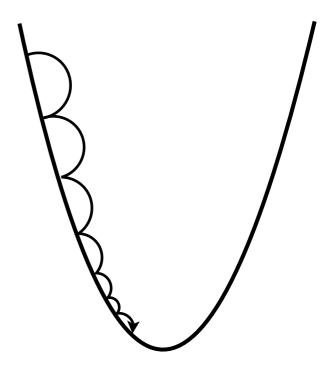
Gradient Descent

Problem:

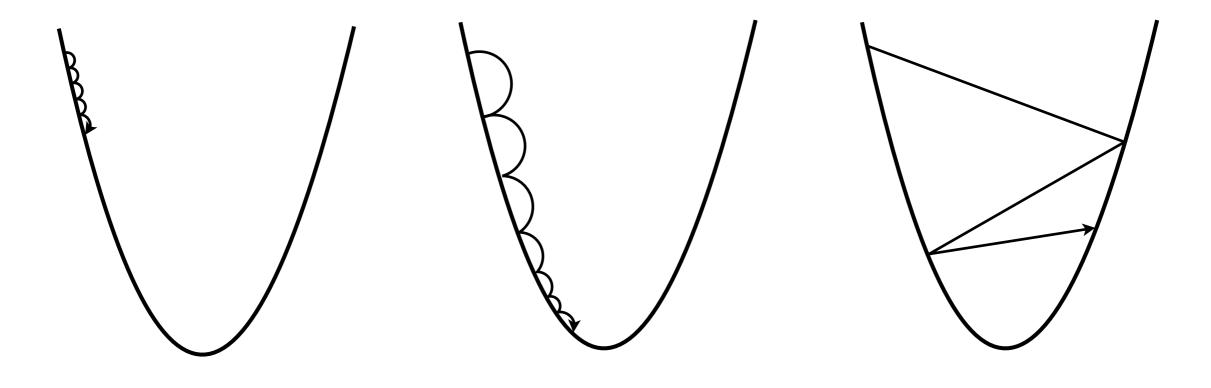
$$\arg\min_{\boldsymbol{w}} f(\boldsymbol{w})$$

 $\begin{array}{ll} \underline{\text{Iterative Solution:}} & \boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \frac{\partial f(\boldsymbol{w})}{\partial \boldsymbol{w}} \\ & \uparrow \end{array}$

Step Size



Step Size Selection



Too Small

Just Right

Too Big

Step Size Selection

<u>Exact Line Search:</u> $\eta^* = \arg \min_{\eta \ge 0} f\left(\boldsymbol{w} - \eta \frac{\partial f(\boldsymbol{w})}{\partial \boldsymbol{w}} \right)$ Most often we cannot obtain a closed-form solution!

<u>Backtracking Line Search</u>: Choose $0 < \beta < 1$, $0 < \alpha < 0.5$ and $\eta_0 \ge 0$ and while:

$$f\left(\boldsymbol{w} - \eta_t \frac{\partial f(\boldsymbol{w})}{\partial \boldsymbol{w}}\right) > f(\boldsymbol{w}) - \alpha \eta_t \left\| \frac{\partial f(\boldsymbol{w})}{\partial \boldsymbol{w}} \right\|_2^2$$
$$\eta_{t+1} = \beta \eta_t$$

set:

We start with a big step size and keep decreasing it until the update generates a sufficient decrease for our function. We want out next iterate to beat the criterion value of a linear approximation of our function at the current point. The above inequality is called the **Armijo rule** and it is often used in combination with a **curvature condition**. Check the <u>wikipedia</u> page on Wolfe conditions for more informations.

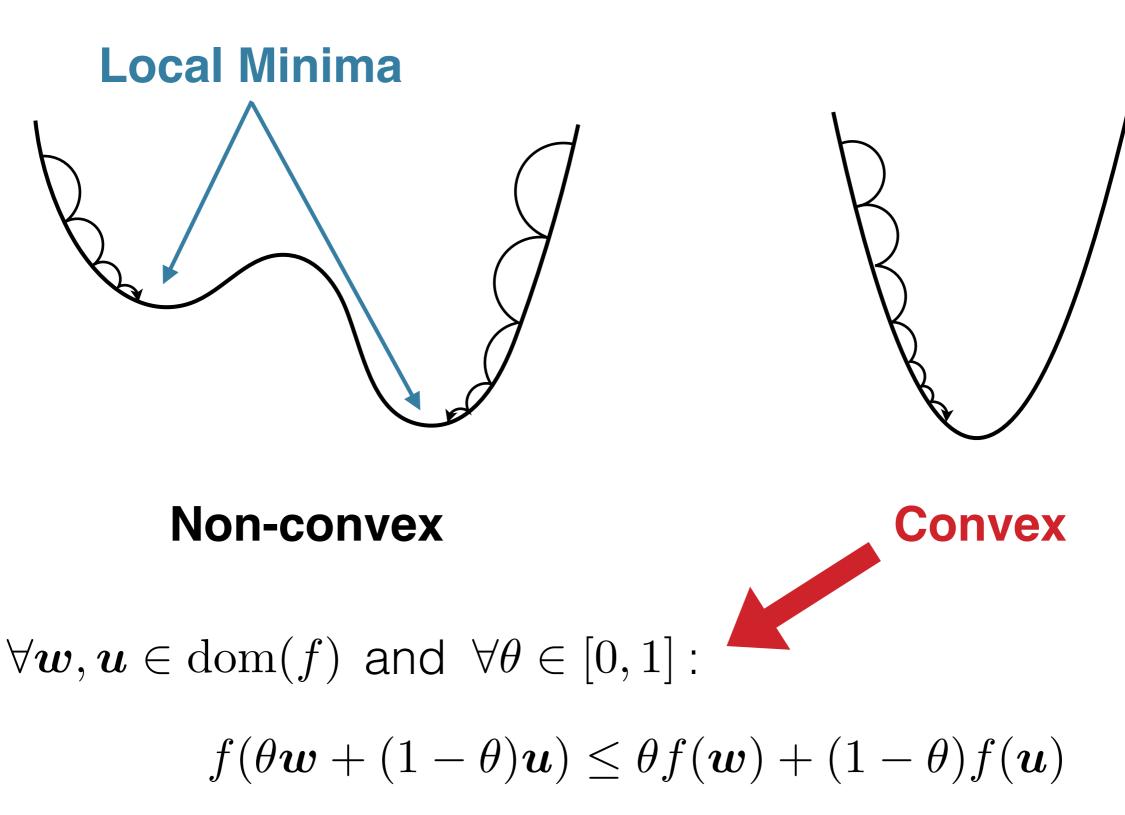
Other Convex Optimization Methods

There are other convex optimization methods that use even second derivative information, such as **Newton's method**. Use the **inverse Hessian** as the step size (makes use of **curvature** information)

> If the Hessian is too expensive to compute, people might also use **quasi-Newton** methods such as the well known **LBFGS** algorithm.

But, what is convexity?

Convexity



Operations that Preserve Convexity

<u>Nonnegative linear combinations</u>: If f_1, \ldots, f_m are convex, then $\alpha_1 f_1 + \cdots + \alpha_m f_m$ is convex for any $\alpha_1, \ldots, \alpha_m \ge 0$.

<u>Affine compositions</u>: If f is convex, then $g(w) = f(\mathbf{A}w + \mathbf{b})$ is also convex.

<u>Pointwise maximum</u>: If f_1, \ldots, f_m are convex, then then max $\{f_1, \ldots, f_m\}$ is also convex.

Back to Logistic Regression

Sum of affine functions and convex functions.

$$\boldsymbol{w} = \arg \max_{\boldsymbol{w}} L(\boldsymbol{w}) = \arg \max_{\boldsymbol{w}} \sum_{i=1}^{n} y^{i}(\boldsymbol{w}^{\top}\boldsymbol{x}^{i}) - \log\left(1 + e^{\boldsymbol{w}^{\top}\boldsymbol{x}^{i}}\right)$$

$$\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} = \sum_{i=1}^{n} \boldsymbol{x}^{i} \left(y^{i} - \frac{e^{\boldsymbol{w}^{\top} \boldsymbol{x}^{i}}}{1 + e^{\boldsymbol{w}^{\top} \boldsymbol{x}^{i}}} \right)$$

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta \frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}}$$

Logistic Regression with a Prior

$$\begin{split} \boldsymbol{w} \sim \mathcal{N}(\boldsymbol{0}, \sigma^{2}\mathbf{I}) & \|\boldsymbol{w}\|_{2}^{2} \triangleq \sum_{j} w_{j}^{2} \\ L(\boldsymbol{w}) = \sum_{i=1}^{n} y^{i}(\boldsymbol{w}^{\top}\boldsymbol{x}^{i}) - \log\left(1 + e^{\boldsymbol{w}^{\top}\boldsymbol{x}^{i}}\right) - \frac{1}{2\sigma^{2}} \|\boldsymbol{w}\|_{2}^{2} \\ \frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} = \sum_{i=1}^{n} \boldsymbol{x}^{i} \left(y^{i} - \frac{e^{\boldsymbol{w}^{\top}\boldsymbol{x}^{i}}}{1 + e^{\boldsymbol{w}^{\top}\boldsymbol{x}^{i}}}\right) - \frac{1}{\sigma^{2}} \boldsymbol{w} \end{split}$$

More generally we call this **L2 regularization**:

$$\arg\min_{\boldsymbol{w}} f(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_2^2$$

Regularization in Optimization

More generally we have **Lp regularization**:

$$\arg\min_{\boldsymbol{w}} f(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_p^p$$

L1 is a special case, frequently used in practice to induce **sparsity** in the solution:

$$\arg\min_{\boldsymbol{w}} f(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_1$$

Stochastic Gradient Descent

We can randomly sample terms of that sum and get an estimate of the gradient in order to speed things up

$$\boldsymbol{w} = \arg \max_{\boldsymbol{w}} L(\boldsymbol{w}) = \arg \max_{\boldsymbol{w}} \sum_{i=1}^{n} y^{i}(\boldsymbol{w}^{\top}\boldsymbol{x}^{i}) - \log\left(1 + e^{\boldsymbol{w}^{\top}\boldsymbol{x}^{i}}\right)$$

$$\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} = \sum_{i=1}^{n} \boldsymbol{x}^{i} \left(y^{i} - \frac{e^{\boldsymbol{w}^{\top} \boldsymbol{x}^{i}}}{1 + e^{\boldsymbol{w}^{\top} \boldsymbol{x}^{i}}} \right)$$

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