Logistic Regression Optimization

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DERIVATION

Slides adapted from Emily Fox

Reminder: Logistic Regression

$$P(Y=0|X) = \frac{1}{1+\exp\left[\beta_0 + \sum_i \beta_i X_i\right]} \tag{1}$$

$$P(Y=1|X) = \frac{\exp\left[\beta_0 + \sum_i \beta_i X_i\right]}{1+\exp\left[\beta_0 + \sum_i \beta_i X_i\right]} \tag{2}$$

- Discriminative prediction: $p(y|x)$
- Classification uses: ad placement, spam detection
- What we didn't talk about is how to learn β from data

Logistic Regression: Objective Function

$$\mathscr{L} \equiv \ln p(Y \mid X, \beta) = \sum_j \ln p(y^{(j)} \mid x^{(j)}, \beta) \tag{3}$$

$$= \sum_j y^{(j)} \left(\beta_0 + \sum_i \beta_i x_i^{(j)} \right) - \ln \left[1 + \exp \left(\beta_0 + \sum_i \beta_i x_i^{(j)} \right) \right] \tag{4}$$

Logistic Regression: Objective Function

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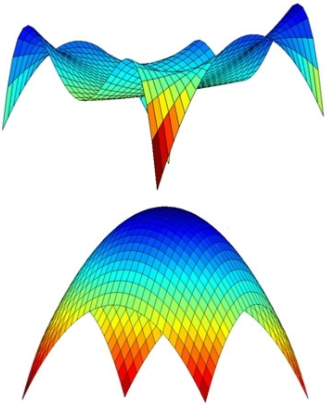
Training data (y, x) are fixed. Objective function is a function of β ... what values of β give a good value.

Convexity



- Convex function
- Doesn’t matter where you start, if you “walk up” objective

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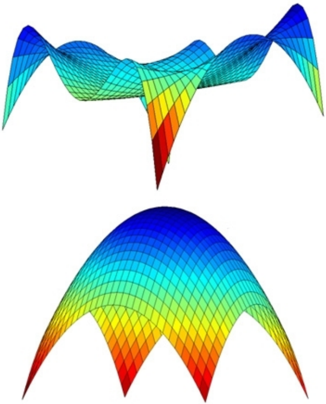
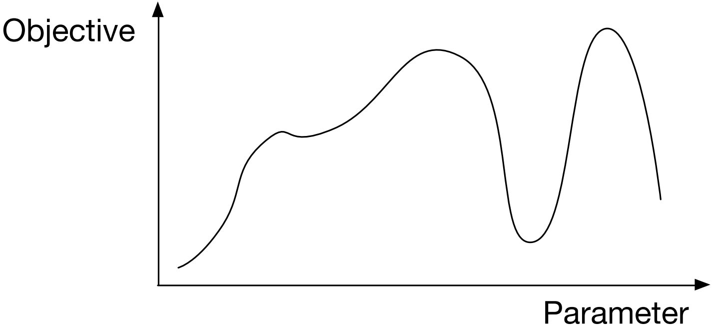


- Convex function
- Doesn't matter where you start, if you "walk up" objective
- Gradient!

Gradient Descent (non-convex)

Goal

Optimize log likelihood with respect to variables β



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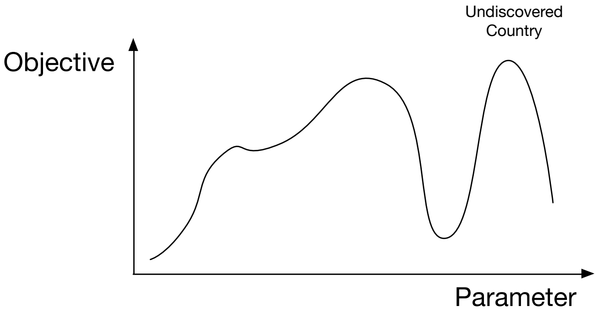

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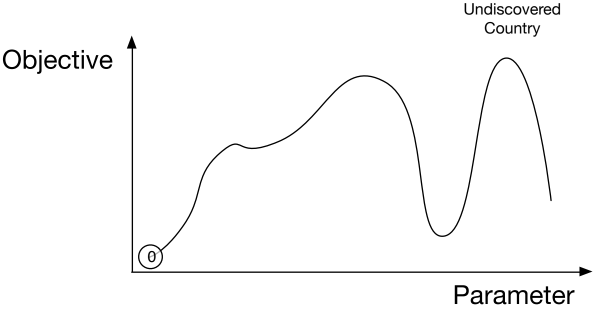

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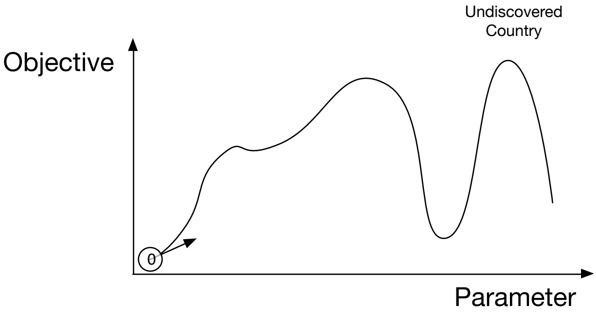

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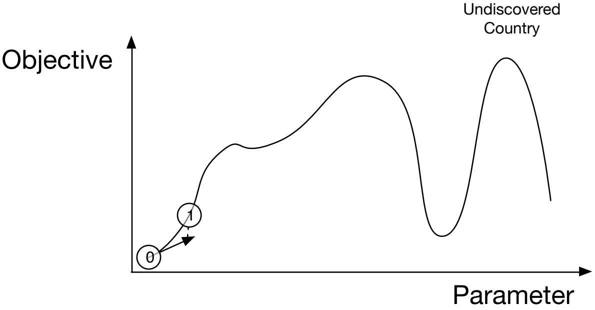

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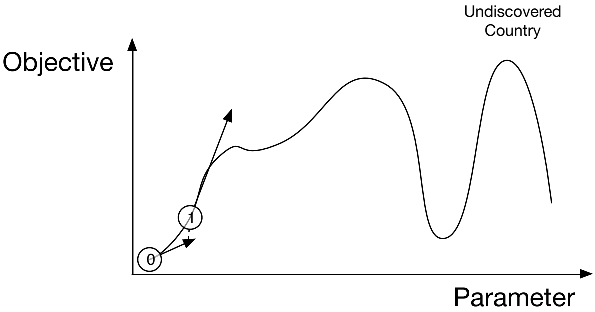

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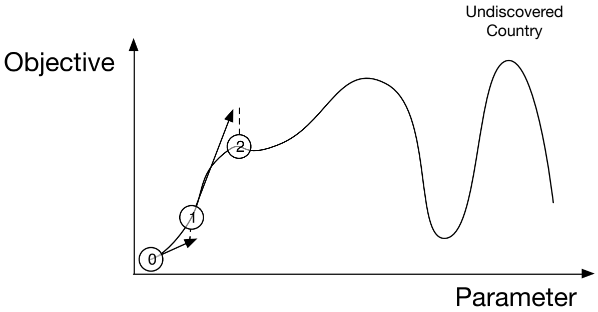

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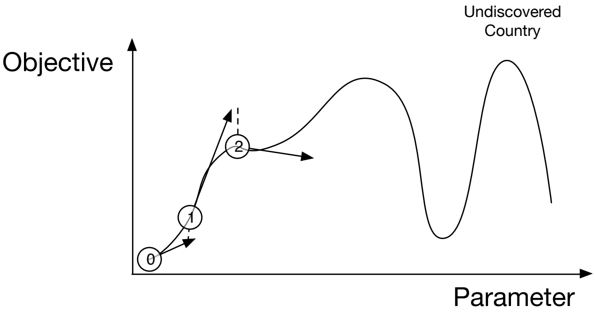

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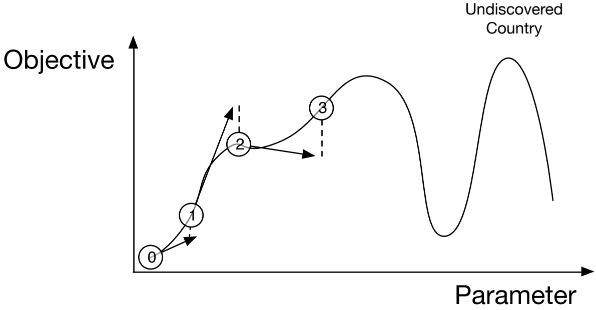

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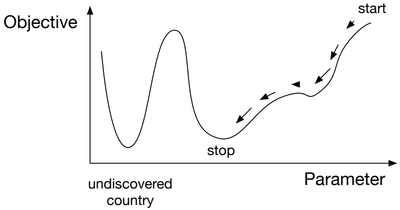

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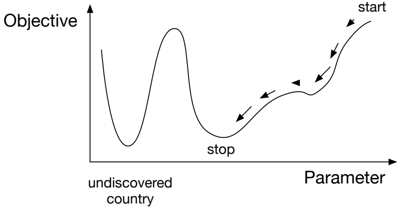

Luckily, (vanilla) logistic regression is convex

Gradient for Logistic Regression

To ease notation, let's define

$$\pi_i = \frac{\exp \beta^T x_i}{1 + \exp \beta^T x_i} \tag{5}$$

Our objective function is

$$\mathscr{L} = \sum_i \log p(y_i \,|\, x_i) = \sum_i \mathscr{L}_i = \sum_i \begin{cases} \log \pi_i & \text{if } y_i = 1 \\ \log(1 - \pi_i) & \text{if } y_i = 0 \end{cases} \tag{6}$$

Taking the Derivative

Apply chain rule:

$$\frac{\partial \mathcal{L}}{\partial \beta_j} = \sum_i \frac{\partial \mathcal{L}_i(\vec{\beta})}{\partial \beta_j} = \sum_i \begin{cases} \frac{1}{\pi_i} \frac{\partial \pi_i}{\partial \beta_j} & \text{if } y_i = 1 \\ \frac{1}{1-\pi_i}\left(-\frac{\partial \pi_i}{\partial \beta_j}\right) & \text{if } y_i = 0 \end{cases} \tag{7}$$

If we plug in the derivative,

$$\frac{\partial \pi_i}{\partial \beta_j} = \pi_i(1-\pi_i)x_j, \tag{8}$$

we can merge these two cases

$$\frac{\partial \mathcal{L}_i}{\partial \beta_j} = (y_i - \pi_i)x_j. \tag{9}$$

Gradient for Logistic Regression

Gradient

$$\nabla_\beta \mathscr{L}(\vec{\beta}) = \left[\frac{\partial \mathscr{L}(\vec{\beta})}{\partial \beta_0}, \dots, \frac{\partial \mathscr{L}(\vec{\beta})}{\partial \beta_n}\right] \quad (10)$$

Update

$$\Delta\beta \equiv \eta \nabla_\beta \mathscr{L}(\vec{\beta}) \quad (11)$$

$$\beta_i' \leftarrow \beta_i + \eta \frac{\partial \mathscr{L}(\vec{\beta})}{\partial \beta_i} \quad (12)$$

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Why are we adding? What would well do if we wanted to do **descent**?

Gradient for Logistic Regression

Gradient

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η: step size, must be greater than zero

Gradient for Logistic Regression

Gradient

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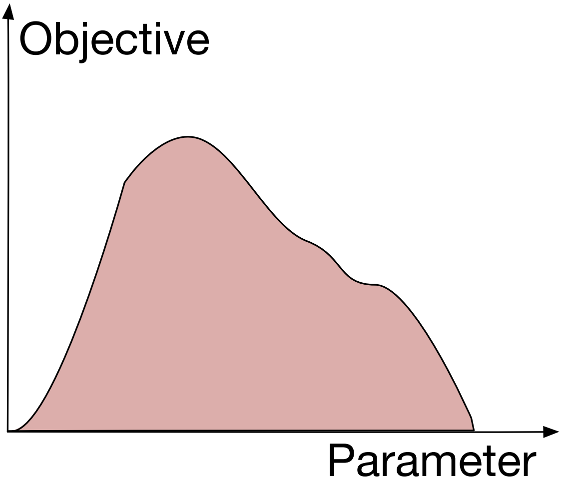
NB: Conjugate gradient is usually better, but harder to implement

Choosing Step Size



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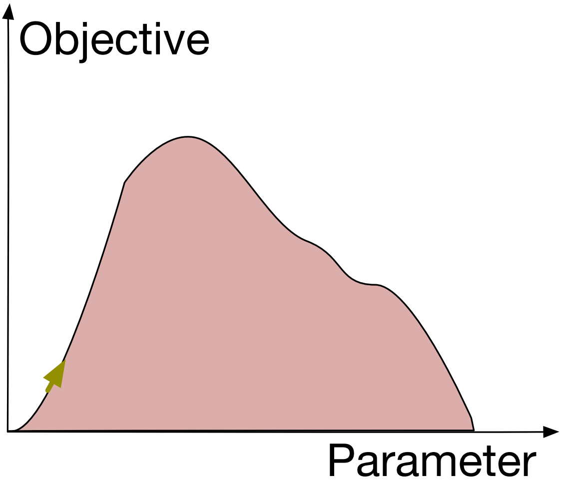

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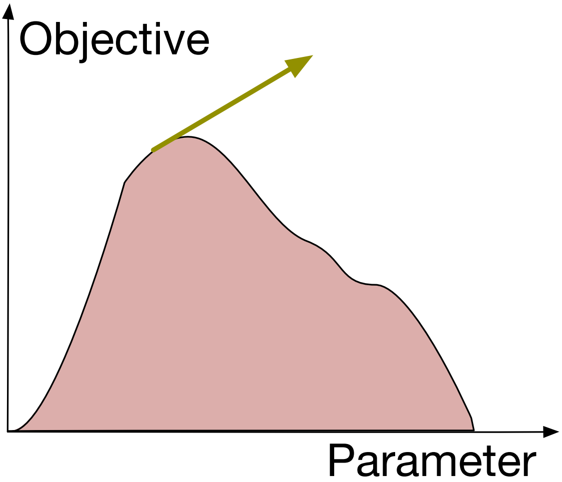

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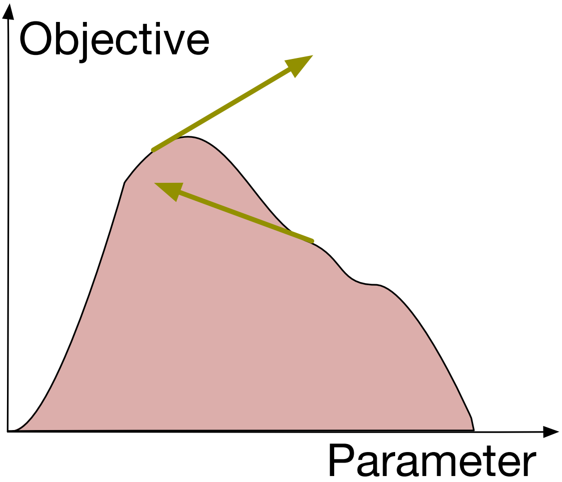

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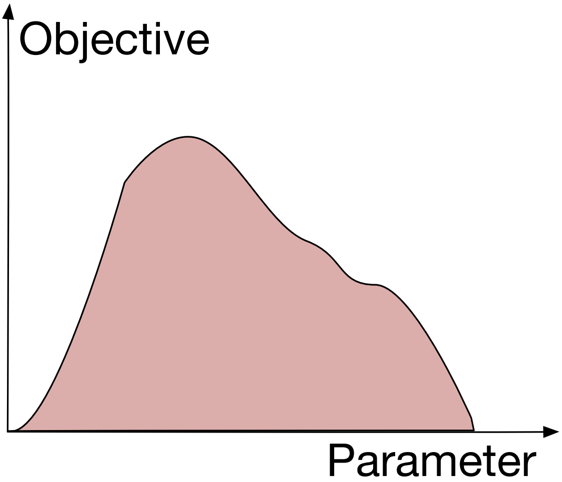

Remaining issues

- When to stop?
- What if β keeps getting bigger?

Regularized Conditional Log Likelihood

Unregularized

$$\beta^* = \arg\max_{\beta} \ln \left[p(y^{(j)} \,|\, x^{(j)}, \beta) \right] \tag{13}$$

Regularized

$$\beta^* = \arg\max_{\beta} \ln \left[p(y^{(j)} \,|\, x^{(j)}, \beta) \right] - \mu \sum_i \beta_i^2 \tag{14}$$

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μ is "regularization" parameter that trades off between likelihood and having small parameters

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- Our datasets are big (to fit into memory)
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- Hard to compute true gradient

$$\mathscr{L}(\beta) \equiv \mathbb{E}_x \left[\nabla \mathscr{L}(\beta, x) \right] \tag{15}$$

- Average over all observations

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- Average over all observations
- What if we compute an update just from one observation?

Getting to Union Station

Pretend it's a pre-smartphone world and you want to get to Union Station

Stochastic Gradient for Logistic Regression

Given a **single observation** x_i chosen at random from the dataset,

$$\beta_j \leftarrow \beta_j' + \eta \left(-\mu \beta_j' + x_{ij} \left[y_i - \pi_i \right] \right) \tag{16}$$

Stochastic Gradient for Logistic Regression

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$$\beta_j \leftarrow \beta'_j + \eta \left(-\mu \beta'_j + x_{ij} \left[y_i - \pi_i \right] \right) \tag{16}$$

Examples in class.

Stochastic Gradient for Regularized Regression

$$\mathscr{L} = \log p(y \mid x; \beta) - \mu \sum_j \beta_j^2 \quad (17)$$

Stochastic Gradient for Regularized Regression

$$\mathscr{L} = \log p(y \,|\, x; \beta) - \mu \sum_j \beta_j^2 \tag{17}$$

Taking the derivative (with respect to example x_i)

$$\frac{\partial \mathscr{L}}{\partial \beta_j} = (y_i - \pi_i) x_j - 2\mu\beta_j \tag{18}$$

Algorithm

1. Initialize a vector B to be all zeros
2. For $t = 1, \ldots, T$
   - For each example $\vec{x}_i, y_i$ and feature j:
     - Compute $\pi_i \equiv \Pr(y_i = 1 \mid \vec{x}_i)$
     - Set $\beta[j] = \beta[j]' + \lambda(y_i - \pi_i)x_i$
3. Output the parameters $\beta_1, \ldots, \beta_d$.

Proofs about Stochastic Gradient

- Depends on convexity of objective and how close ϵ you want to get to actual answer
- Best bounds depend on changing η over time and **per dimension** (not all features created equal)

In class

- Your questions!
- Working through simple example
- Prepared for logistic regression homework