CEE 616: Probabilistic Machine Learning

Foundations: Optimization

Jimi Oke

UMass Amherst

College of Engineering

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Outline

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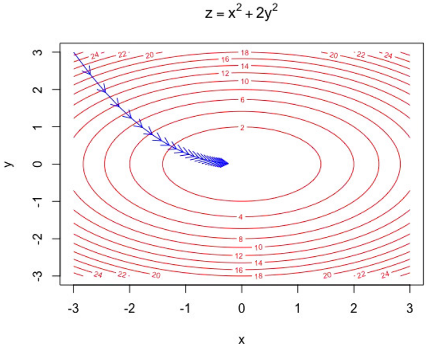

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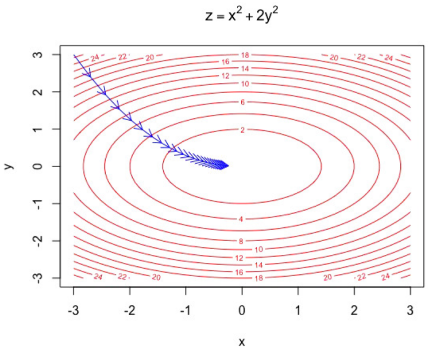

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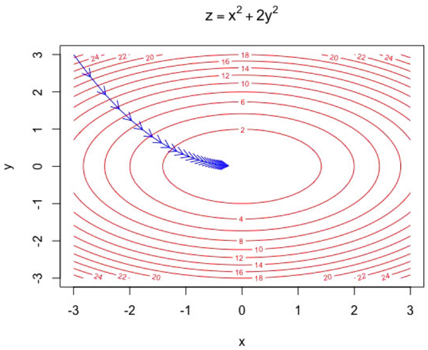

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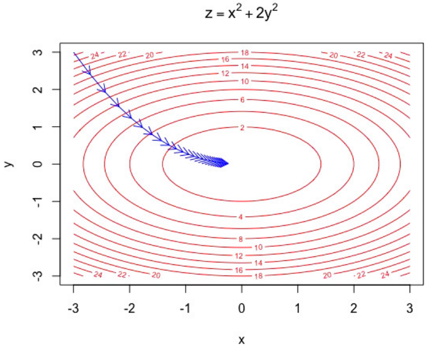

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- First-order methods (e.g. gradient descent)
- Second-order methods (e.g. Newton's method)

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- Begin with an initial value $\boldsymbol{\theta}_0$
- At each iteration t, update $\boldsymbol{\theta}_{t+1}$
- Terminate when $\mathcal{L}(\boldsymbol{\theta}_{t+1}) - \mathcal{L}(\boldsymbol{\theta}_t) = \epsilon$

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The classic first-order method is **gradient descent**

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- Sequence $\{\rho_t\}$ in an optimization algorithm is known as the learning rate schedule

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We choose $\lambda = 0.05$ and a random starting point between 0 and 1.

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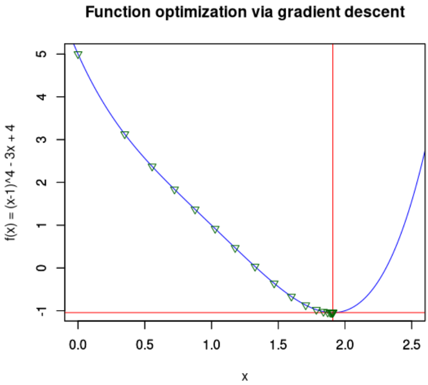

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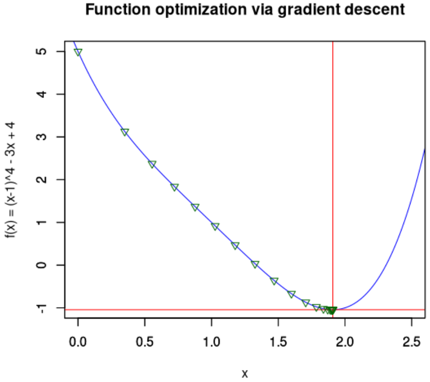

Using the `gradient-descent.ipynb` notebook, we find the optimal point as $\mathbf{(1.908, -1.044)}$. How does the learning rate impact the solution process?

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This approach introduces additional computational expense

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where $c \in [0, 1]$ is typically chosen as 10^{-4}

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This method is also called **Nesterov accelerated gradient**

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- Finite sum: $\mathcal{L}(\boldsymbol{\theta}_t) = \frac{1}{N}\sum_{n=1}^{N} \mathcal{L}_n(\boldsymbol{\theta}_t)$

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Thus, we set the descent diretion $\boldsymbol{d}_t$ as $-\boldsymbol{H}_t^{-1}\boldsymbol{g}_t$

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BFGS

Broyden-Fletcher-Goldfarb-Shanno method. Approximates $\boldsymbol{H}_t \approx \boldsymbol{B}_t$:

$$\boldsymbol{B}_{t+1} = \boldsymbol{B}_t + \frac{\boldsymbol{y}_t \boldsymbol{y}_t^\top}{\boldsymbol{y}_t^\top \boldsymbol{s}_t} - \frac{(\boldsymbol{B}_t \boldsymbol{s}_t)(\boldsymbol{B}_t \boldsymbol{s}_t)^\top}{\boldsymbol{s}_t^\top \boldsymbol{B}_t \boldsymbol{s}_t} \tag{32}$$

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- $\boldsymbol{B}_0$ is typically intialized as $\boldsymbol{I}$ (positive definite)
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- The update can be reduced to a recurrence relation that depends explicitly on $\boldsymbol{C}_0$ and the history of $\boldsymbol{s}_t$ and $\boldsymbol{y}_t$
- For computational efficiency, the M most recent $\boldsymbol{s}_t$, $\boldsymbol{y}_t$ may be used instead
- M is typically $\in [5, 20]$
- This approach is termed L-BFGS (limited memory BFGS)

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And the MLE's would be found by simultaneously solving the partial derivatives set to 0 for each parameter.

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We can use either Newton-Raphson or gradient *ascent* to *maximize* ℓ.

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- However, it may require more iterations to converge than Newton-Raphson

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$$\begin{pmatrix} \beta_{0,k+1} \\ \beta_{1,k+1} \end{pmatrix} = \begin{pmatrix} \beta_{0,k} \\ \beta_{1,k} \end{pmatrix} - \left[\begin{pmatrix} \frac{\partial^2 \ell(\beta)}{\partial {\beta_0}^2} & \frac{\partial^2 \ell(\beta)}{\partial \beta_0 \partial \beta_1} \\ \frac{\partial^2 \ell(\beta)}{\partial \beta_1 \partial \beta_0} & \frac{\partial^2 \ell(\beta)}{\partial {\beta_1}^2} \end{pmatrix}^{-1} \begin{pmatrix} \frac{\partial \ell}{\partial \beta_0} \\ \frac{\partial \ell}{\partial \beta_1} \end{pmatrix} \right]_{\beta_k} \tag{51}$$

Alternatively:

Newton-Raphson approach for MLE (cont.)

We can work out each component of the second derivative:

$$\frac{\partial^2 \ell(\beta)}{\partial {\beta_0}^2} = -\sum_i p(x_i)(1 - p(x_i)) \tag{48}$$

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Alternatively:

$$\beta_{k+1} = \beta_k - \left[\left(\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} \right)^{-1} \frac{\partial \ell(\beta)}{\partial \beta} \right]_{\beta_k} \tag{52}$$

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- Complementary slackness: $\boldsymbol{\mu} \odot \boldsymbol{g} = \mathbf{0}$

Further topics

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- Linear programming (simplex algorithm)
- Quadratic programming
- Proximal gradient method
- Bound optimization (majorize-minimize algorithms)
- Expectation maximization (EM); for MLE/MAP estimation

Reading assignments

- **PMLI** 8
- **PMLCE** 5