Numerical Optimization

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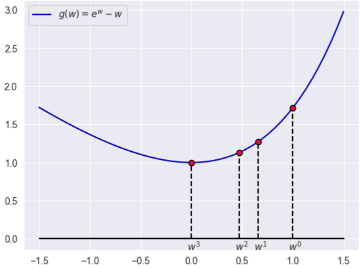
3. Repeat Step (2) – converging to a stationary point, in good scenario – until you meet a **stopping condition** at some step T. The approximate stationary point (potentially a minimizer) is $\mathbf{w}^{(T)}$.



Outline

Gradient Descent

Newton's method - a second-order method

Examples and some convergence guarantees

Gradient Descent - a first-order method

Looking to minimize a loss (cost) function $\ell : \mathbb{R}^N \to \mathbb{R}$. Want to approximate stationary point for ℓ in $\mathbb{R}^N$, in order to minimize ℓ (hopefully).

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- choose a ("small") threshhold value ε. Stop when, as part of the last update, the change in every parameter divided by its size is not more than ε. That is, stop when

$$\frac{|\omega_j^{(t)} - \omega_j^{(t-1)}|}{|\omega_j^{(t-1)}|} \leq \varepsilon, \qquad \forall 1 \leq j \leq p.$$

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Note: linear approximation is

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How does one change $\mathbf{w}^{(t)}$ to make $h(\mathbf{w})$ decrease the most? Want some (fixed length vector) $\Delta\mathbf{w}$ so that $h(\mathbf{w}^{(t)}) - h(\mathbf{w}^{(t)} + \Delta\mathbf{w})$ is as large as possible.

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Since

$$h(\mathbf{w}^{(t)}) - h(\mathbf{w}^{(t)} + \Delta \mathbf{w}) = -\nabla \ell(\mathbf{w}^{(t)})^T \Delta \mathbf{w}$$

this occurs when $\nabla \ell(\mathbf{w}^{(t)})^T \Delta \mathbf{w}$ is as negative as possible, which is when $\Delta \mathbf{w}$ is in the opposite direction of $\nabla \ell(\mathbf{w}^{(t)})$; and so, our update is $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \Delta \mathbf{w} = \mathbf{w}^{(t)} - \alpha_{t+1} \nabla \ell(\mathbf{w}^{(t)})$.

Convergence

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Short answer: No, not necessarily.

...so, *in what cases* can we guarantee such a thing?

Issues with convergence

To demonstrate the difficulty, imagine a "toy" loss function: $\ell : \mathbb{R} \to \mathbb{R}$ with $\ell(w) = w^2$. At each w we have $\nabla \ell = \left(\frac{d\ell}{dw} \right) = (2w)$.

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Say learning rate: $\alpha_{t+1} > 1$ for all t. Then, at any $w^{(t)} > 0$, we get

$$w^{(t+1)} = w^{(t)} - 2\alpha_{t+1} w^{(t)} < w^{(t)} - 2w^{(t)} = -w^{(t)},$$

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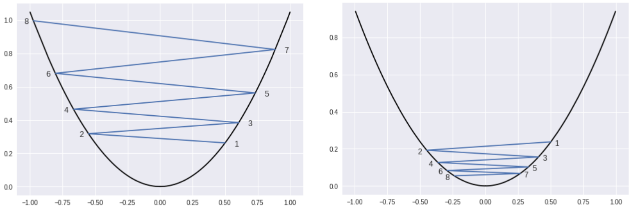

Figure: Gradient descent on $\ell(w) = w^2$. Left: $\alpha = 1.05$; right: $\alpha = 0.95$.

Outline

Newton's method

As before, we want to use approximations to get closer to a stationary point of $\ell : \mathbb{R}^N \to \mathbb{R}$, however we will now use a second order approximation:

$$h(\mathbf{w}) = \ell(\mathbf{w}^{(t)}) + \nabla \ell(\mathbf{w}^{(t)})^T(\mathbf{w} - \mathbf{w}^{(t)}) + \frac{1}{2}(\mathbf{w} - \mathbf{w}^{(t)})^T \nabla^2 \ell(\mathbf{w}^{(t)})(\mathbf{w} - \mathbf{w}^{(t)}).$$

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As a consequence from the recent homework, this has a stationary point at a solution to the linear equation $\nabla^2 \ell(\mathbf{w}^{(t)})\mathbf{w} = \nabla^2 \ell(\mathbf{w}^{(t)})\mathbf{w}^{(t)} - \nabla \ell(\mathbf{w}^{(t)})$. Call that solution $\mathbf{w}^{(t+1)}$. Repeat the above step until some stopping condition is met.

Newton's method - advantages and disadvantages

Advantage: When converging to a minimum of the function, Newton's method will converge in fewer steps.
Disadvantages: One has to compute the Hessian – more computation time and more storage needed. Solving the linear system can also have numerical issues and take more time.
Also, if ℓ is not convex (and $\mathbf{w}^{(t)}$ is not in a convex region for the function), then it may approach a maximum instead of minimum.

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Example with Linear regression

Last time: given sample data $\mathcal{S}$ for simple linear regression, and using MSE as empirical loss, $\mathcal{L}_{\mathcal{S}}(m, b) = \frac{1}{n}\sum_{i=1}^{n}(mx_i + b - y_i)^2$, we found

$$\nabla \mathcal{L}_{\mathcal{S}}(m, b) = \left(\frac{2}{n}\sum_{i=1}^{n}(mx_i + b - y_i)x_i, \quad \frac{2}{n}\sum_{i=1}^{n}(mx_i + b - y_i) \right).$$

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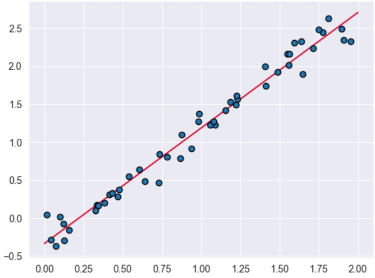
Example: batch gradient descent working on the `'Example1.csv'` data.

The LSR line, using closed form.

- $\hat{m} \approx 1.520$, $\hat{b} = -0.3346$:



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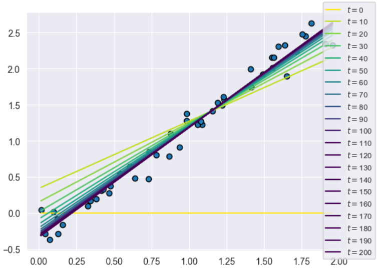

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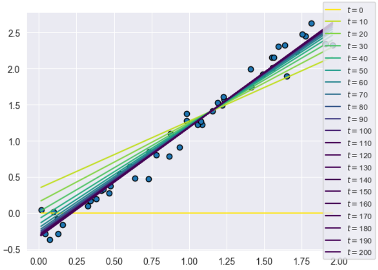
Plot of selected lines found during batch GD updates; starting parameters $m = 0$, $b = 0$; learning rate set to 0.1. Parameter values on iteration 208: $m = 1.519$, $b = -0.334$.



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```
## lr is learning rate; threshhold is for stopping;
input: X, y, lr, threshhold
p ← initial array of parameters
while (max of last_update > threshhold){
    grad ← compute_grad(p, X, y)
    last_update ← | grad / p | ## entrywise array division
    # handle p[i] near 0
    p ← p − lr*grad
}
return p
```

Guarantees of convergence

If your loss function is differentiable and a **convex function**, and if have some "control" on size of the gradient then, by choosing η small enough, can guarantee convergence.

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Theorem

Suppose that $\mathcal{L} : \mathbb{R}^p \to \mathbb{R}$ is differentiable and convex, and suppose that $\nabla \mathcal{L}$ is Lipschitz continuous[2] with some constant $C > 0$ and that $\eta \leq 1/C$. Then, for a minimizer ω^* of $\mathcal{L}$,

$$\mathcal{L}(\omega^{(t)}) - \mathcal{L}(\omega^*) \leq \frac{|\omega^{(0)} - \omega^*|^2}{2\eta t}.$$

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- The difference between $\mathcal{L}(\omega^{(t)})$ and the minimum of $\mathcal{L}$ is bounded by a constant times $1/t$.

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Previous theorem requires using actual gradient of $\mathcal{L}$ in each update step. Here is a convergence guarantee that allows for a random vector $\mathbf{D}_t$, in place of $\nabla\mathcal{L}$, as long as $\mathbb{E}\big[\mathbf{D}_t \big| \omega^{(t)}\big] = \nabla\mathcal{L}\big(\omega^{(t)}\big)$.

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Theorem

Suppose that $\mathcal{L}$ is differentiable and convex, that $\omega^{(0)} = \mathbf{0}$, and that $\eta = \frac{1}{\sqrt{K}}$ for an integer $K > 0$. Finally, suppose that $\left|\mathbf{D}_t\right| \leq 1$ for all $1 \leq t \leq K$. Then, for a minimizer ω^* of $\mathcal{L}$,

$$\mathbb{E}[\mathcal{L}(\bar{\omega})] - \mathcal{L}(\omega^*) \leq \frac{1}{\sqrt{K}}$$

where $\bar{\omega}$ is the average of $\omega^{(1)}, \omega^{(2)}, \ldots, \omega^{(K)}$.