Optimization in Machine Learning

First order methods
Gradient descent

Learning goals

- Iterative Descent / Line Search
- Descent directions
- GD
- ERM with GD
- Pseudoresiduals

ITERATIVE DESCENT

Let f be the height of a mountain depending on the geographic coordinates (x_1, x_2)

$$f : \mathbb{R}^2 \to \mathbb{R}, \quad f(x_1, x_2) = y.$$

Goal: Reach the valley

$$\arg\min_{\mathbf{x}} f(\mathbf{x})$$

Central idea: Repeat

1. At current location $\mathbf{x} \in \mathbb{R}^d$ search for **descent direction** $\mathbf{d} \in \mathbb{R}^d$
2. Move along $\mathbf{d}$ until f „sufficiently“ reduces (**step size control**) and update location

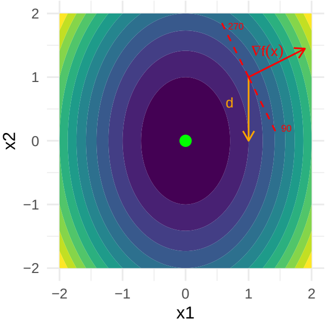
"Walking down the hill, towards the valley."

ITERATIVE DESCENT

Let $f : \mathbb{R}^d \to \mathbb{R}$ continuously differentiable.

Definition: $\mathbf{d} \in \mathbb{R}^d$ is a descent direction in $\mathbf{x}$ if

$$D_{\mathbf{d}} f(\mathbf{x}) = \nabla f(\mathbf{x})^T \mathbf{d} < 0 \text{ (neg. directional derivative)}$$



Angle between $\nabla f(\mathbf{x})$ and $\mathbf{d}$ must be $\in (90^\circ, 270^\circ)$.

ITERATIVE DESCENT / 2

Algorithm Iterative Descent / Line search

1: Starting point $\mathbf{x}^{[0]} \in \mathbb{R}^d$
2: **while** Stopping criterion not met **do**
3: Calculate a descent direction $\mathbf{d}^{[t]}$ for current $\mathbf{x}^{[t]}$
4: Find $\alpha^{[t]}$ s.t. $f(\mathbf{x}^{[t+1]}) < f(\mathbf{x}^{[t]})$ for $\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} + \alpha^{[t]}\mathbf{d}^{[t]}$.
5: Update $\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} + \alpha^{[t]}\mathbf{d}^{[t]}$
6: **end while**

NB: Terminology is sometimes ambiguous: “line search” can refer to Step 4 (selecting the step size that decreases $f(\mathbf{x})$) and can mean umbrella term for iterative descent algorithms.

Key questions:

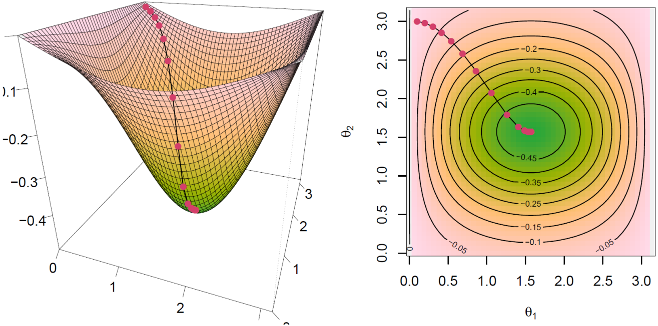
- How to choose $\mathbf{d}^{[t]}$ (now)
- How to choose $\alpha^{[t]}$ (later)

GRADIENT DESCENT

Properties of gradient:

- $\nabla f(\mathbf{x})$: direction of greatest increase
- $-\nabla f(\mathbf{x})$: direction of greatest decrease

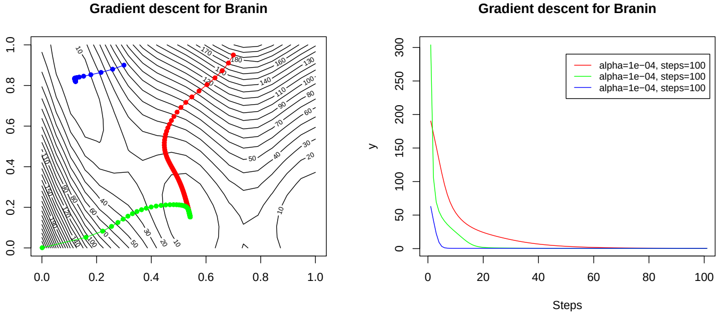
Using $\mathbf{d} = -\nabla f(\mathbf{x})$ is called **gradient descent**.



GD for $f(x_1, x_2) = -\sin(x_1) \cdot \frac{1}{2\pi} \exp\left((x_2 - \pi/2)^2\right)$ with sensibly chosen step size $\alpha^{[t]}$.

GD AND MULTIMODAL FUNCTIONS

Outcome will depend on start point.



100 iters of GD with const $\alpha = 10^{-4}$.

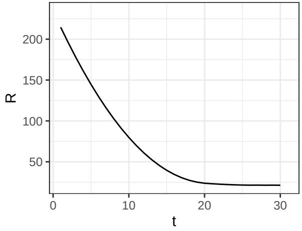
OPTIMIZE LS LINEAR REGRESSION WITH GD

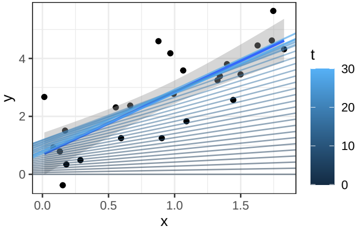
Let $\mathcal{D} = \left(\left(\mathbf{x}^{(1)}, y^{(1)}\right), \ldots, \left(\mathbf{x}^{(n)}, y^{(n)}\right)\right)$ and minimize

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(\boldsymbol{\theta}^{\top}\mathbf{x}^{(i)} - y^{(i)}\right)^2$$

NB: For illustration, we use GD even though closed-form solution exists. GD-like (more adv.) approaches like this MIGHT make sense for large data, though.

Gradient: $$\nabla_{\boldsymbol{\theta}}\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \frac{\partial \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = -\sum_{i=1}^{n} 2 \cdot \left(y^{(i)} - \boldsymbol{\theta}^{\top}\mathbf{x}^{(i)}\right)\mathbf{x}^{(i)}$$



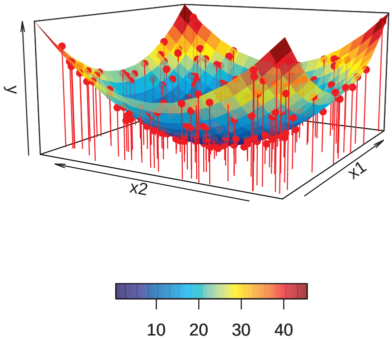


ERM FOR NN WITH GD

Let $\mathcal{D} = \left(\left(\mathbf{x}^{(1)}, y^{(1)}\right), \dots, \left(\mathbf{x}^{(n)}, y^{(n)}\right) \right)$, with $y = x_1^2 + x_2^2$ and minimize

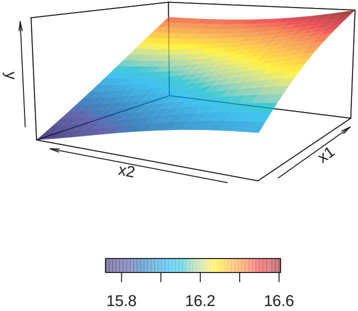
$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(f(\mathbf{x} \mid \boldsymbol{\theta}) - y^{(i)} \right)^2$$

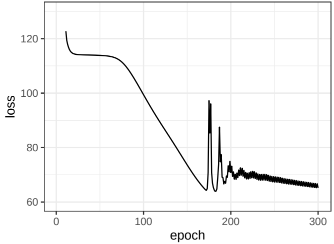
where $f(\mathbf{x} \mid \boldsymbol{\theta})$ is a neural network with 2 hidden layers (2 units each).

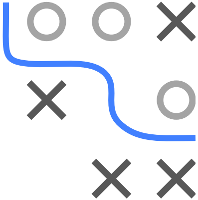


ERM FOR NN WITH GD / 2

After 10 iters of GD:

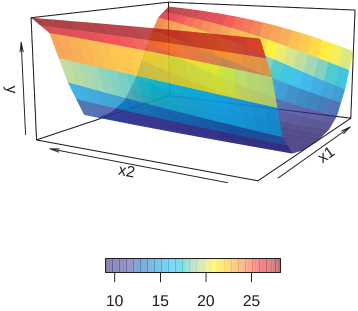


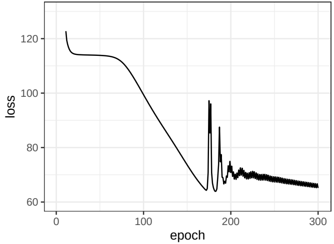




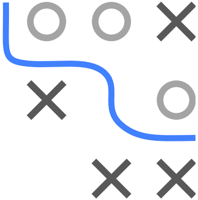
ERM FOR NN WITH GD / 3

After 100 iters of GD:

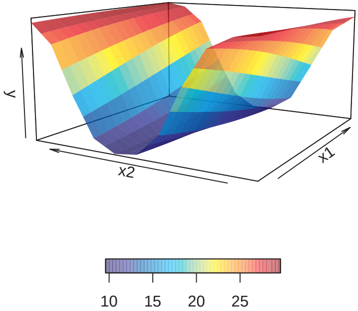


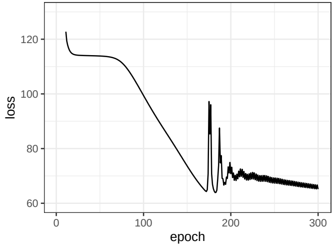


ERM FOR NN WITH GD / 4



After 300 iters of GD (note the zig-zag-behavior after iter. 200):





GD FOR ERM: PSEUDORESIDUALS

Gradient for ERM problem:

$$-\frac{\partial \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = -\frac{\partial \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)}{\partial \boldsymbol{\theta}} = -\sum_{i=1}^{n} \underbrace{\frac{\partial L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)}{\partial f}}_{\text{pseudo residual } \tilde{r}^{(i)}(f)} \frac{\partial f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)}{\partial \boldsymbol{\theta}}$$

- **pseudo residuals** tell us how to distort $f\left(\mathbf{x}^{(i)}\right)$ to achieve greatest decrease of $L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$ (best pointwise update)
- $\frac{\partial f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)}{\partial \boldsymbol{\theta}}$ tells us how to modify $\boldsymbol{\theta}$ accordingly and wiggle model output
- GD step sums up these modifications across all observations i

NB: Pseudo-residuals $\tilde{r}(f)$ match usual residuals for L2 loss:

$$\frac{\partial L\left(y, f(\mathbf{x})\right)}{\partial f} = \frac{1}{2} \left.\frac{\partial (y-f)^2}{\partial f}\right|_{f=f(\mathbf{x})} = y - f(\mathbf{x})$$