

Optimization

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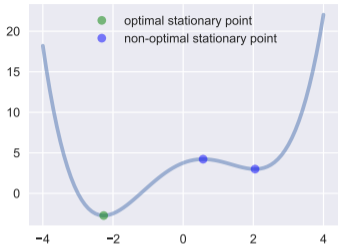
Optimization problems and algorithms

Optimization problem

minimize $f(\theta)$

- ▶ $\theta \in \mathbf{R}^d$ is the *variable* or *decision variable*
- ▶ $f : \mathbf{R}^d \rightarrow \mathbf{R}$ is the *objective function*
- ▶ goal is to choose θ to minimize f
- ▶ θ^* is *optimal* means that for all θ , $f(\theta) \geq f(\theta^*)$
- ▶ $f^* = f(\theta^*)$ is the *optimal value* of the problem
- ▶ optimization problems arise in many fields and applications, including machine learning

Optimality condition



- ▶ let's assume that f is *differentiable*, i.e., partial derivatives $\frac{\partial f(\theta)}{\partial \theta_i}$ exist
- ▶ if θ^* is optimal, then $\nabla f(\theta^*) = 0$
- ▶ $\nabla f(\theta) = 0$ is called the *optimality condition* for the problem
- ▶ there can be points that satisfy $\nabla f(\theta) = 0$ but are not optimal
- ▶ we call points that satisfy $\nabla f(\theta) = 0$ *stationary points*
- ▶ not all stationary points are optimal

Solving optimization problems

- ▶ in some cases, we can solve the problem analytically
- ▶ e.g., least squares: minimize $f(\theta) = \|X\theta - y\|_2^2$
 - ▶ optimality condition is $\nabla f(\theta) = 2X^T(X\theta - y) = 0$
 - ▶ this has (unique) solution $\theta^* = (X^T X)^{-1} X^T y = X^\dagger y$
(when columns of X are linearly independent)
- ▶ in other cases, we resort to an *iterative algorithm* that computes a sequence $\theta^1, \theta^2, \dots$ with, hopefully, $f(\theta^k) \rightarrow f^*$ as $k \rightarrow \infty$

Iterative algorithms

▶ *iterative algorithm* computes a sequence $\theta^1, \theta^2, \dots$

▶ θ^k is called the k th *iterate*

▶ θ^1 is called the *starting point*

▶ many iterative algorithms are *descent methods*, which means

$$f(\theta^{k+1}) < f(\theta^k), \quad k = 1, 2, \dots$$

i.e., each iterate is better than the previous one

▶ this means that $f(\theta^k)$ converges, but not necessarily to f^*

Stopping criterion

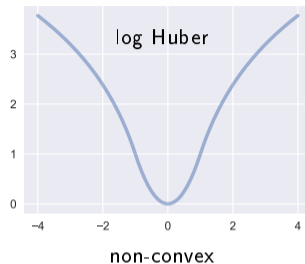
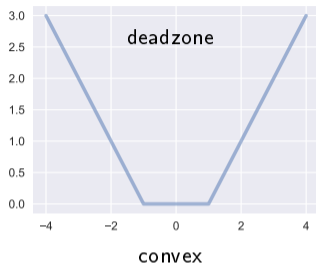
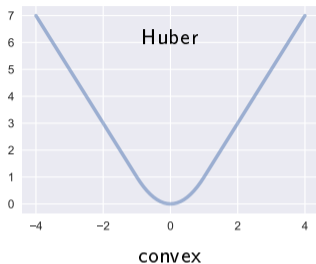
- ▶ in practice, we stop after a finite number K of steps
- ▶ typical stopping criterion: stop if $\|\nabla f(\theta^k)\|_2 \leq \epsilon$ or $k = k^{\max}$
- ▶ ϵ is a small positive number, the *stopping tolerance*
- ▶ k^{\max} is the maximum number of iterations
- ▶ in words: we stop when θ^k is almost a stationary point
- ▶ we hope that $f(\theta^K)$ is not too much bigger than f^*
- ▶ or more realistically, that θ^K is at least useful for our application

Non-heuristic and heuristic algorithms

- ▶ in some cases we *know* that $f(\theta^k) \rightarrow f^*$, for any θ^1
- ▶ in words: *we'll get to a solution if we keep iterating*
- ▶ called *non-heuristic*

- ▶ other algorithms do not guarantee that $f(\theta^k) \rightarrow f^*$
- ▶ we can hope that even if $f(\theta^k) \not\rightarrow f^*$, θ^k is still useful for our application
- ▶ called *heuristic*

Convex functions



- ▶ a function $f : \mathbf{R}^d \rightarrow \mathbf{R}$ is *convex* if for any θ , $\tilde{\theta}$, and α with $0 \leq \alpha \leq 1$,

$$f(\alpha\theta + (1 - \alpha)\tilde{\theta}) \leq \alpha f(\theta) + (1 - \alpha)f(\tilde{\theta})$$

- ▶ roughly speaking, f has 'upward curvature'
- ▶ for $d = 1$, same as $f''(\theta) \geq 0$ for all θ

Convex optimization

- ▶ optimization problem

$$\text{minimize } f(\theta)$$

is called *convex* if the objective function f is convex

- ▶ for convex optimization problem, $\nabla f(\theta) = 0$ only for θ optimal, *i.e.*,
all stationary points are optimal

- ▶ algorithms for convex optimization are non-heuristic
- ▶ *i.e.*, *we can solve convex optimization problems* (exactly, in principle)

Convex ERM problems

- ▶ linear prediction model $\hat{y} = \theta^\top x$
- ▶ regularized empirical risk function $f(\theta) = \mathcal{L}(\theta) + \lambda r(\theta)$, with $\lambda \geq 0$,

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^n p(\theta^\top x^i - y^i), \quad r(\theta) = q(\theta_1) + \cdots + q(\theta_d)$$

- ▶ f is convex if loss penalty p and parameter penalty q functions are convex

- ▶ convex penalties: square, absolute, tilted absolute, Huber, logistic
- ▶ non-convex penalties: log Huber, squareroot

Gradient method

Gradient method

- ▶ assume f is differentiable
- ▶ at iteration θ^k , create affine (Taylor) approximation of f valid near θ^k

$$\hat{f}(\theta; \theta^k) = f(\theta^k) + \nabla f(\theta^k)^T (\theta - \theta^k)$$

- ▶ $\hat{f}(\theta; \theta^k) \approx f(\theta)$ for θ near θ^k
- ▶ choose θ^{k+1} to make $\hat{f}(\theta^{k+1}; \theta^k)$ small, but with $\|\theta^{k+1} - \theta^k\|_2$ not too large
- ▶ choose θ^{k+1} to minimize $\hat{f}(\theta; \theta^k) + \frac{1}{2h^k} \|\theta - \theta^k\|_2^2$
- ▶ $h^k > 0$ is a *trust parameter* or *step length* or *learning rate*
- ▶ solution is $\theta^{k+1} = \theta^k - h^k \nabla f(\theta^k)$
- ▶ roughly: take step in direction of negative gradient

Gradient method update

- ▶ choose θ^{k+1} to as minimizer of

$$f(\theta^k) + \nabla f(\theta^k)^T (\theta - \theta^k) + \frac{1}{2h^k} \|\theta - \theta^k\|_2^2$$

- ▶ rewrite as

$$f(\theta^k) + \frac{1}{2h^k} \|(\theta - \theta^k) + h^k \nabla f(\theta^k)\|_2^2 - \frac{h^k}{2} \|\nabla f(\theta^k)\|_2^2$$

- ▶ first and third terms don't depend on θ
- ▶ middle term is minimized (made zero!) by choice

$$\theta = \theta^k - h^k \nabla f(\theta^k)$$

How to choose step length

- ▶ if h^k is too large, we can have $f(\theta^{k+1}) > f(\theta^k)$
- ▶ if h^k is too small, we have $f(\theta^{k+1}) < f(\theta^k)$ but progress is slow

- ▶ a simple scheme:
 - ▶ if $f(\theta^{k+1}) > f(\theta^k)$, set $h^{k+1} = h^k/2$, $\theta^{k+1} = \theta^k$ (a *rejected step*)
 - ▶ if $f(\theta^{k+1}) \leq f(\theta^k)$, set $h^{k+1} = 1.2h^k$ (an *accepted step*)
- ▶ reduce step length by half if it's too long; increase it 20% otherwise

Gradient method summary

choose an initial $\theta^1 \in \mathbf{R}^d$ and $h^1 > 0$ (e.g., $\theta^1 = 0$, $h^1 = 1$)

for $k = 1, 2, \dots, k^{\max}$

1. compute $\nabla f(\theta^k)$; quit if $\|\nabla f(\theta^k)\|_2$ is small enough
2. form tentative update $\theta^{\text{tent}} = \theta^k - h^k \nabla f(\theta^k)$
3. if $f(\theta^{\text{tent}}) \leq f(\theta^k)$, set $\theta^{k+1} = \theta^{\text{tent}}$, $h^{k+1} = 1.2h^k$
4. else set $h^k := 0.5h^k$ and go to step 2

Gradient method convergence

- ▶ (assuming some technical conditions hold) we have

$$\|\nabla f(\theta^k)\|_2 \rightarrow 0 \text{ as } k \rightarrow \infty$$

- ▶ *i.e.*, the gradient method always finds a stationary point

- ▶ for *convex problems*

- ▶ gradient method is *non-heuristic*

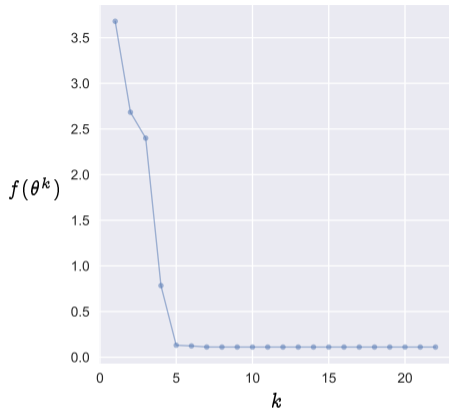
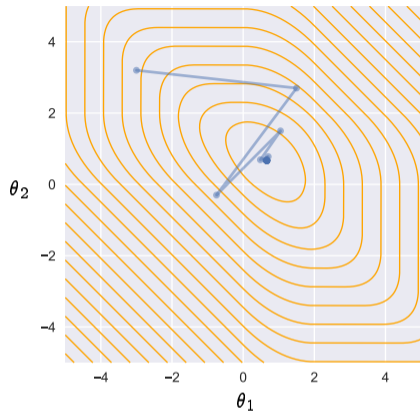
- ▶ for any starting point θ^1 , $f(\theta^k) \rightarrow f^*$ as $k \rightarrow \infty$

- ▶ for *non-convex problems*

- ▶ gradient method is *heuristic*

- ▶ we can (and often do) have $f(\theta^k) \not\rightarrow f^*$

Example: Convex objective

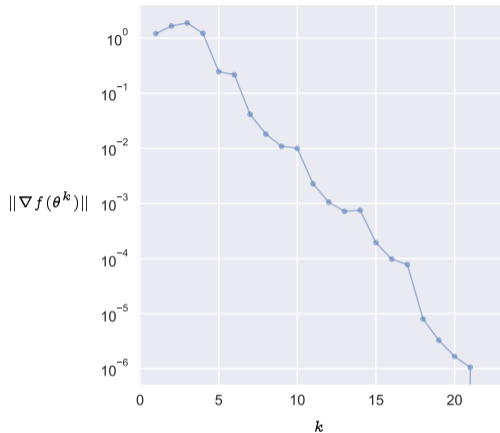
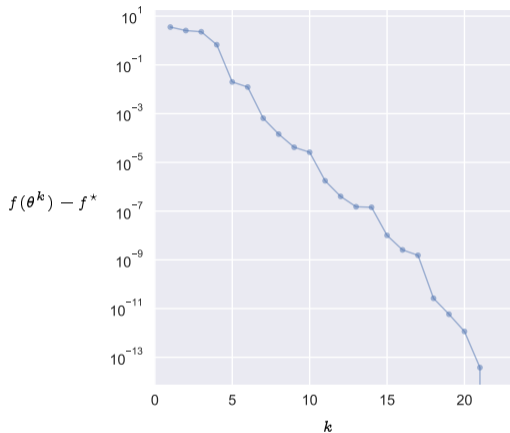


► $f(\theta) = \frac{1}{3}(p^{\text{hub}}(\theta_1 - 1) + p^{\text{hub}}(\theta_2 - 1) + p^{\text{hub}}(\theta_1 + \theta_2 - 1))$

► f is convex

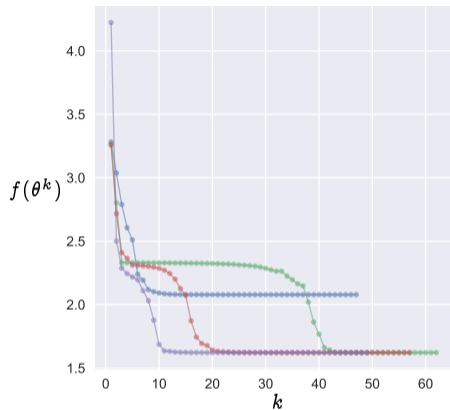
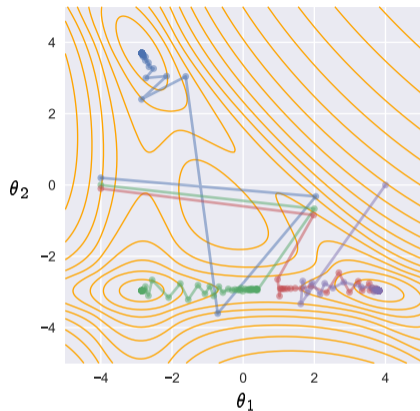
► optimal point is $\theta^* = (2/3, 2/3)$, with $f^* = 1/9$

Example: Convex objective



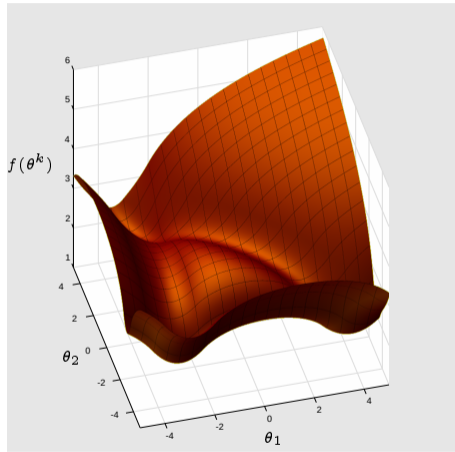
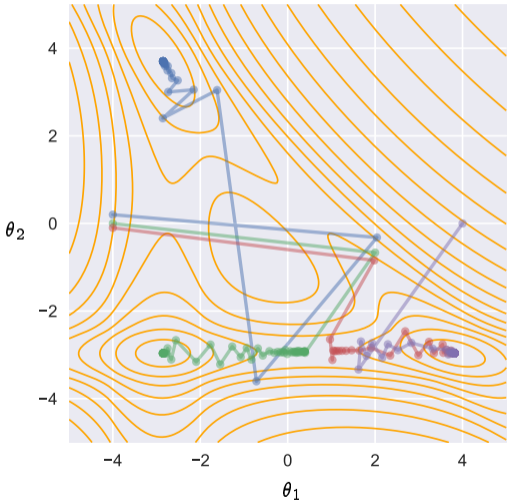
- ▶ $f(\theta^k)$ is a decreasing function of k , (roughly) exponentially
- ▶ $\|\nabla f(\theta^k)\| \rightarrow 0$ as $k \rightarrow \infty$

Example: Non-convex objective

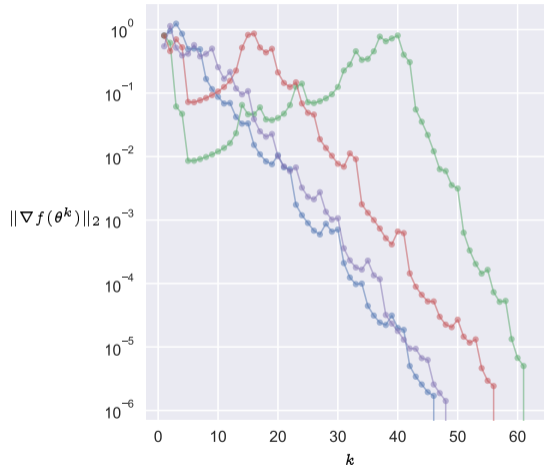
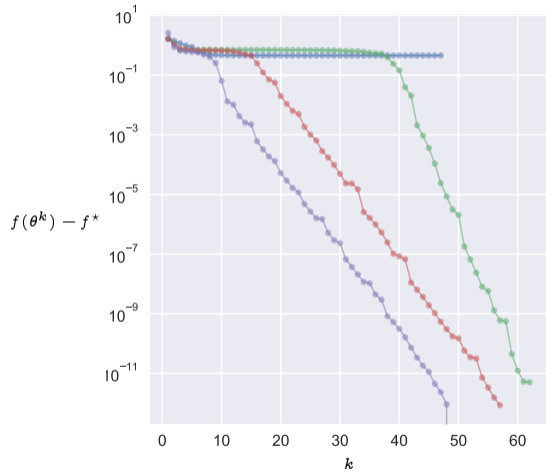


- ▶ $f(\theta) = \frac{1}{3}(p^{\text{lh}}(\theta_1 + 3) + p^{\text{lh}}(2\theta_2 + 6) + p^{\text{lh}}(\theta_1 + \theta_2 - 1))$
- ▶ f is sum of log-Huber functions, so not convex
- ▶ gradient algorithm converges, but limit depends on initial guess

Example: Non-convex objective



Example: Non-convex objective



Gradient method for ERM

Gradient of empirical risk function

- ▶ predictor is $\hat{y} = g_{\theta}(x)$; we consider case of scalar y
- ▶ empirical risk is sum of terms for each data point

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(\hat{y}^i, y^i) = \frac{1}{n} \sum_{i=1}^n \ell(g_{\theta}(x^i), y^i)$$

- ▶ convex if loss function ℓ is convex in first argument and predictor is linear, i.e., $g_{\theta}(x) = \theta^T x$
- ▶ gradient is sum of terms for each data point

$$\nabla \mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell'(g_{\theta}(x^i), y^i) \nabla g_{\theta}(x^i)$$

- ▶ $\ell'(\hat{y}, y)$ is derivative of ℓ with respect to its first argument \hat{y}
- ▶ $\nabla g_{\theta}(x)$ is the gradient of $g_{\theta}(x)$ with respect to θ

Evaluating gradient of empirical risk function

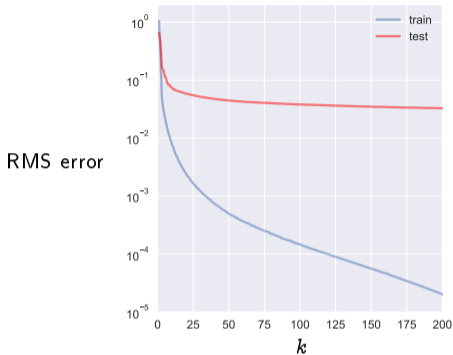
- ▶ assume linear predictor, $g_{\theta}(x) = \theta^{\top}x$, so $\nabla g_{\theta}(x) = x$
- ▶ gradient is

$$\nabla \mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell'(\theta^{\top}x^i, y^i)x^i$$

- ▶ compute n -vector $\hat{y}^k = X\theta^k$
- ▶ compute n -vector z^k , with entries $z_i^k = \ell'(\hat{y}_i^k, y^i)$
- ▶ compute d -vector $\nabla \mathcal{L}(\theta^k) = (1/n)X^T z^k$

- ▶ first and third steps are matrix-vector multiplication, each costing $2nd$ flops
- ▶ second step costs order n flops (dominated by other two)
- ▶ total is $4nd$ flops

Validation



- ▶ can evaluate performance measure on train and test data sets as gradient method runs
- ▶ predictor is often good enough well before gradient descent has converged
- ▶ optimization is only a surrogate for what we want (*i.e.*, a predictor that predicts well on unseen data)