Basics of Numerical Optimization: Iterative Methods

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Computer Science & Engineering
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Find global minimum

1st-order necessary condition: Assume f is 1st-order differentiable at $\boldsymbol{x}_0$. If $\boldsymbol{x}_0$ is a local minimizer, then $\nabla f(\boldsymbol{x}_0) = \mathbf{0}$.

$\boldsymbol{x}$ with $\nabla f(\boldsymbol{x}) = \mathbf{0}$: **1st-order stationary point** (1OSP)

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2nd-order necessary condition: Assume $f(\boldsymbol{x})$ is 2-order differentiable at $\boldsymbol{x}_0$. If $\boldsymbol{x}_0$ is a local min, $\nabla f(\boldsymbol{x}_0) = \mathbf{0}$ and $\nabla^2 f(\boldsymbol{x}_0) \succeq \mathbf{0}$.

$\boldsymbol{x}$ with $\nabla f(\boldsymbol{x}) = \mathbf{0}$ and $\nabla^2 f(\boldsymbol{x}) \succeq \mathbf{0}$: **2nd-order stationary point** (2OSP)

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- **Analytic method**: find 1OSP's using gradient first, then study them using Hessian — for simple functions! e.g., $f(\boldsymbol{x}) = \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2$, or $f(x, y) = x^2y^2 - x^3y + y^2 - 1$)

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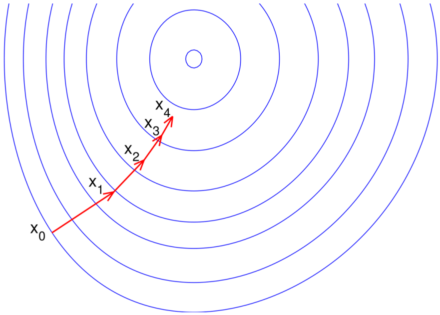
- **Grid search**: incurs $O\left(\varepsilon^{-n}\right)$ cost
- **Iterative methods**: find 1OSP's/2OSP's by making consecutive small movements

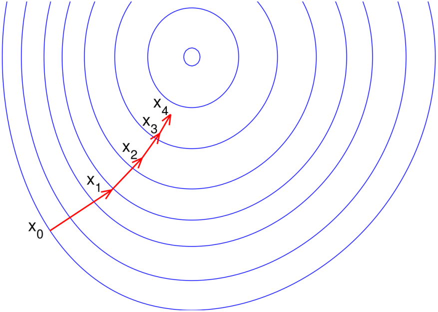
Iterative methods



Credit: aria42.com

Illustration of iterative methods on the contour/levelset plot (i.e., the function assumes the same value on each curve)

Iterative methods



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Two questions: what direction to move, and how far to move

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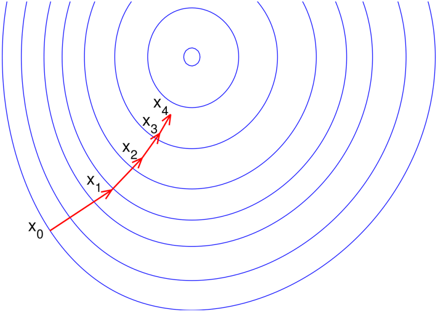

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Two possibilities:

- **Line-search methods**: direction first, size second

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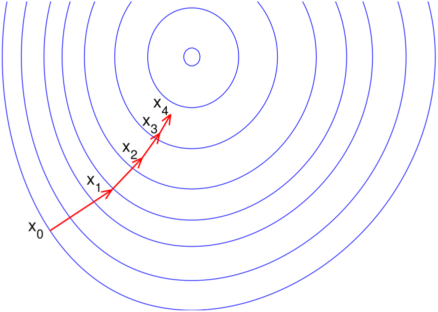

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- **Line-search methods**: direction first, size second
- **Trust-region methods**: size first, direction second

Outline

Framework of line-search methods

A generic line search algorithm

Input: initialization $\boldsymbol{x}_0$, stopping criterion (SC), $k = 1$

```
while SC not satisfied do
    choose a direction d_k
    decide a step size t_k
    make a step: x_k = x_{k-1} + t_k d_k
    update counter: k = k + 1
end while
```

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Input: initialization $\boldsymbol{x}_0$, stopping criterion (SC), $k = 1$

while SC not satisfied **do**
    choose a direction $\boldsymbol{d}_k$
    decide a step size t_k
    make a step: $\boldsymbol{x}_k = \boldsymbol{x}_{k-1} + t_k \boldsymbol{d}_k$
    update counter: $k = k + 1$
end while

Four questions:

- How to choose direction $\boldsymbol{d}_k$?
- How to choose step size t_k?
- Where to initialize?
- When to stop?

How to choose a search direction?

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shortsighted answer: find a direction to decrease most rapidly

for any fixed $t > 0$, using 1st order Taylor expansion

$$f\left(\boldsymbol{x}_k + t\boldsymbol{d}_{k+1}\right) - f\left(\boldsymbol{x}_k\right) \approx t\left\langle \nabla f\left(\boldsymbol{x}_k\right), \boldsymbol{d}_{k+1}\right\rangle$$

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$$\min_{\|\boldsymbol{v}\|_2 = 1} \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{v} \rangle$$

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$$\min_{\|\boldsymbol{v}\|_2 = 1} \left\langle \nabla f\left(\boldsymbol{x}_k\right), \boldsymbol{v}\right\rangle \implies \boldsymbol{v} = -\frac{\nabla f\left(\boldsymbol{x}_k\right)}{\left\|\nabla f\left(\boldsymbol{x}_k\right)\right\|_2}$$

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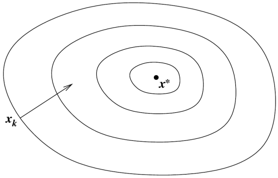

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Set $\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k)$

gradient/steepest descent: $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - t\nabla f(\boldsymbol{x}_k)$

Gradient descent

$$\min_{\boldsymbol{x}} \ \boldsymbol{x}^\top \boldsymbol{A} \boldsymbol{x} + \boldsymbol{b}^\top \boldsymbol{x}$$

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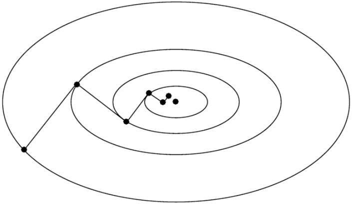
typical zig-zag path



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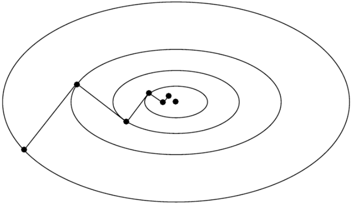
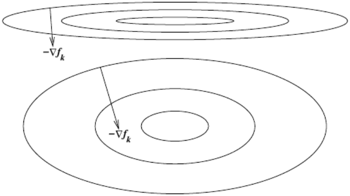


conditioning affects the path length



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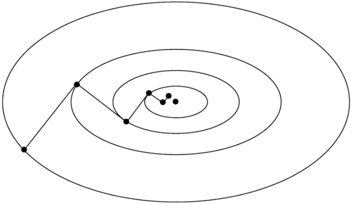

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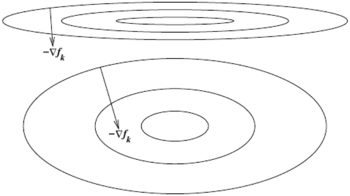
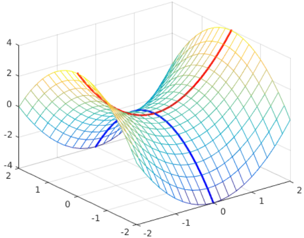


$f(x,y) = x^2 - y^2$



– remember direction curvature?
$\boldsymbol{v}^\intercal \nabla^2 f(\boldsymbol{x})\, \boldsymbol{v} = \frac{d^2}{dt^2} f(\boldsymbol{x} + t\boldsymbol{v})$

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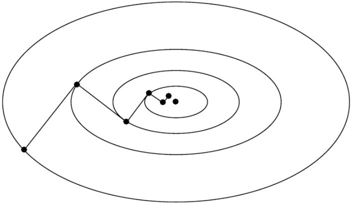

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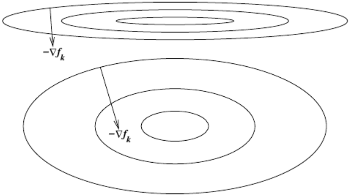

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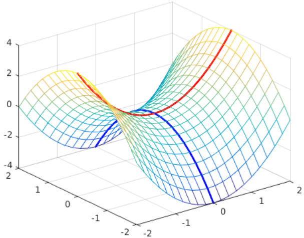

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  $\boldsymbol{v}^\intercal \nabla^2 f(\boldsymbol{x}) \boldsymbol{v} = \frac{d^2}{dt^2} f(\boldsymbol{x} + t\boldsymbol{v})$
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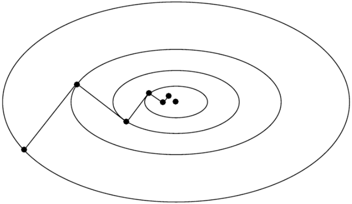

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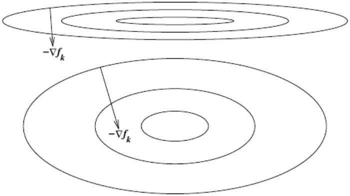

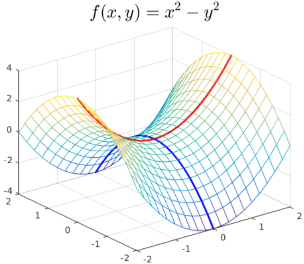

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- directional curvatures encoded in the Hessian

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$$

minimizing the right side

$\Longrightarrow \boldsymbol{v} = -t^{-1} \left[\nabla^2 f\left(\boldsymbol{x}_k\right)\right]^{-1} \nabla f\left(\boldsymbol{x}_k\right)$

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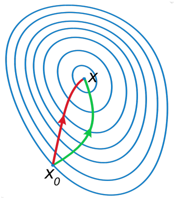

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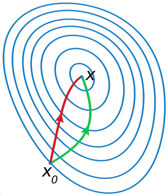

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Set $\boldsymbol{d}_k = \left[\nabla^2 f(\boldsymbol{x}_k)\right]^{-1} \nabla f(\boldsymbol{x}_k)$

Newton's method: $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - t \left[\nabla^2 f(\boldsymbol{x}_k)\right]^{-1} \nabla f(\boldsymbol{x}_k)$,

t can set to be 1.

Why called Newton's method?

Newton's method: $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - t\left[\nabla^2 f\left(\boldsymbol{x}_k\right)\right]^{-1} \nabla f\left(\boldsymbol{x}_k\right)$,

Recall Newton's method for root-finding

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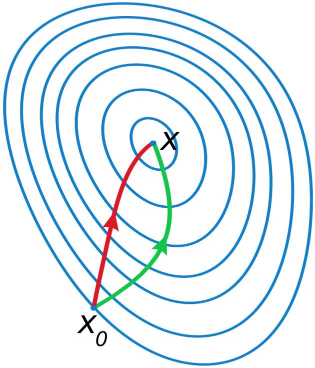

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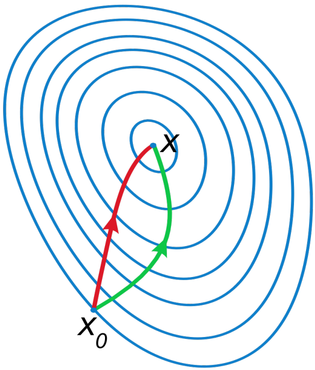

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nearsighted choice: cost $O(n)$ per step

gradient/steepest descent:
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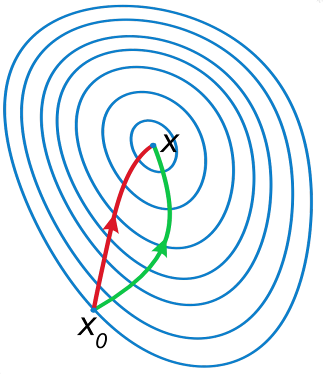

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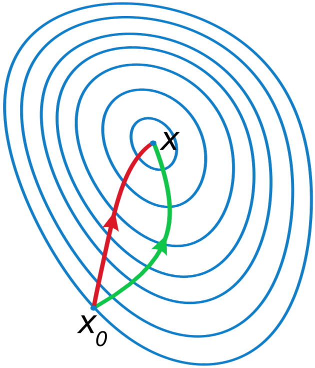

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Implication: The plain Newton never used for large-scale problems. More on this later ...

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solution: e.g., modify the Hessian $\nabla^2 f\left(\boldsymbol{x}_k\right) + \tau \boldsymbol{I}$ with τ sufficiently large

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- **details**: start from $t = 1$. If the **key condition** not satisfied, $t = \rho t$ for a chosen parameter $\rho \in (0,1)$.

Back-tracking line search

A widely implemented strategy in numerical optimization packages

---

Back-tracking line search

Input: initial $t > 0$, $\rho \in (0,1)$, $c \in (0,1)$

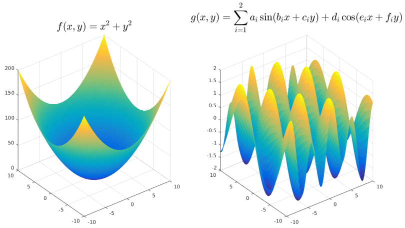
1: **while** $f(\boldsymbol{x}_k + t\boldsymbol{d}_k) - f(\boldsymbol{x}_k) \geq ct \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{d}_k \rangle$ **do**

2: $\quad t = \rho t$

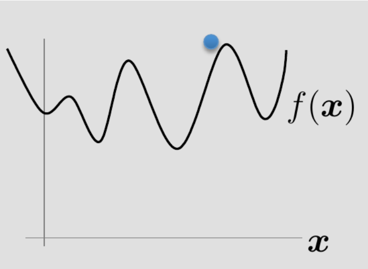
3: **end while**

Output: $t_k = t$.

Where to initialize?



convex vs. nonconvex functions



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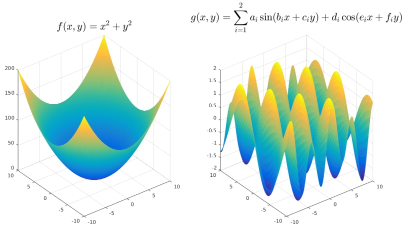

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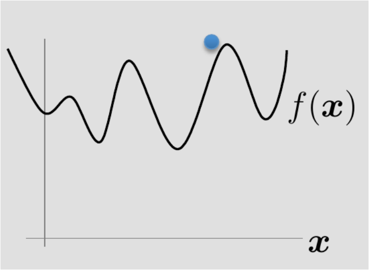

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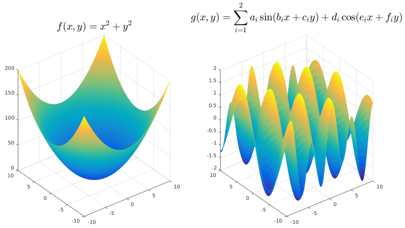

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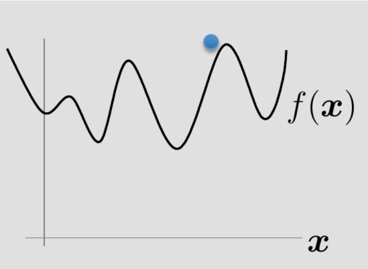

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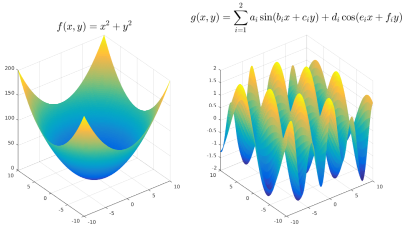

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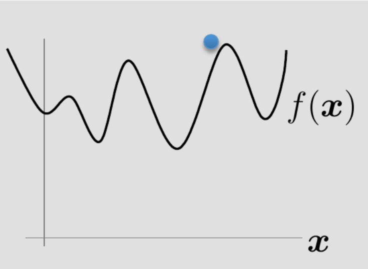

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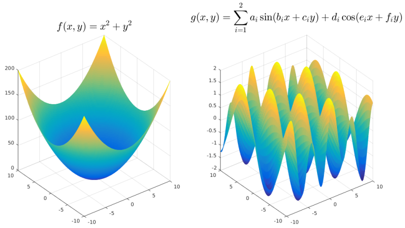

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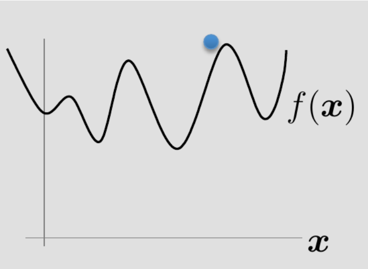

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  https://sunju.org/research/nonconvex/

  and sometimes random initialization works!

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Nonconvex optimization is hard

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(see, e.g., [Murty and Kabadi, 1987])

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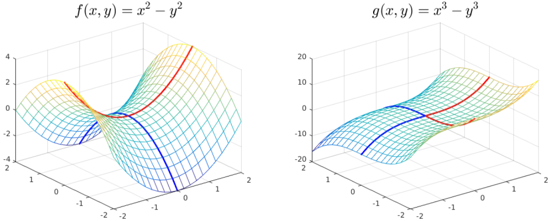

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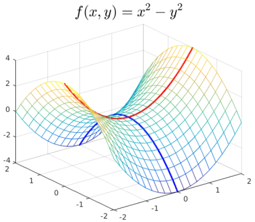
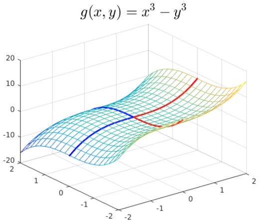


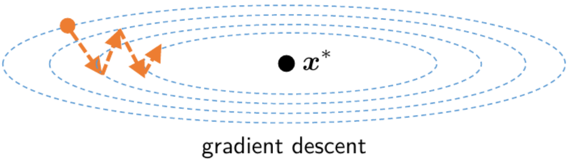


Cases in between: local shapes around SOSP determined by **spectral properties of higher-order derivative tensors**, calculating which is hard [Hillar and Lim, 2013]!

Outline

Outline

Why momentum?



Credit: Princeton ELE522

- GD is cheap ($O(n)$ per step) but overall convergence sensitive to conditioning
- Newton's convergence is not sensitive to conditioning but expensive ($O(n^3)$ per step)

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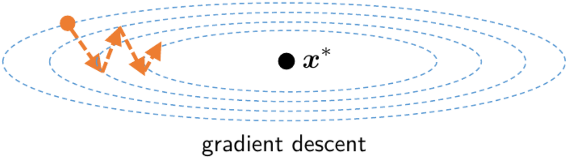

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A cheap way to achieve faster convergence?

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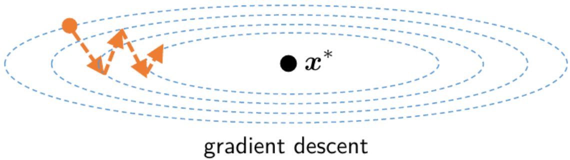

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A cheap way to achieve faster convergence? Answer: using historic information

Heavy ball method

In physics, a heavy object has a large inertia/momentum — resistance to change velocity.

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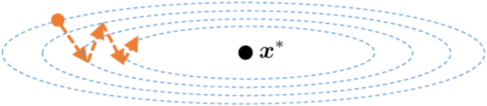
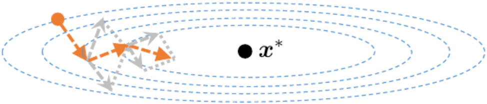


gradient descent



heavy-ball method

Credit: Princeton ELE522

History helps to smooth out the zig-zag path!

Nesterov's accelerated gradient methods

Another version, due to Y. Nesterov

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \beta_k \left(\boldsymbol{x}_k - \boldsymbol{x}_{k-1}\right) - \alpha_k \nabla f \left(\boldsymbol{x}_k + \beta_k \left(\boldsymbol{x}_k - \boldsymbol{x}_{k-1}\right)\right)$$

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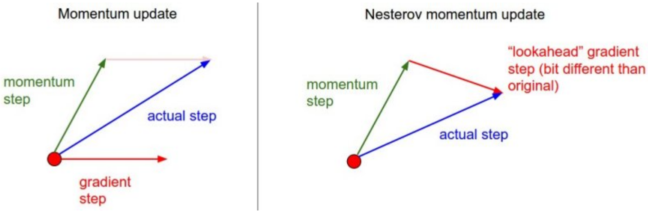

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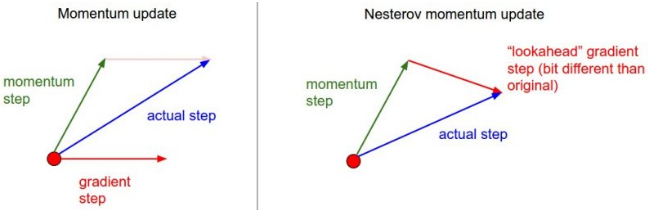

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For more info, see Chap 10 of [Beck, 2017] and Chap 2 of [Nesterov, 2018].

Outline

Quasi-Newton methods

quasi-: seemingly; apparently but not really.

Newton's method: cost $O(n^2)$ storage and $O(n^3)$ computation per step

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - t\left[\nabla^2 f\left(\boldsymbol{x}_k\right)\right]^{-1} \nabla f\left(\boldsymbol{x}_k\right)$$

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Choose $\boldsymbol{H}_k$ to approximate $\nabla^2 f\left(\boldsymbol{x}_k\right)$ so that

- avoid calculation of second derivatives
- simplify matrix inversion, i.e., computing the search direction

Quasi-Newton methods

given: starting point $x_0 \in \mathrm{dom}\, f$, $H_0 \succ 0$

for $k = 0, 1, \ldots$

1. compute quasi-Newton direction $\Delta x_k = -H_k^{-1} \nabla f(x_k)$
2. determine step size t_k (*e.g.*, by backtracking line search)
3. compute $x_{k+1} = x_k + t_k \Delta x_k$
4. compute H_{k+1}

- Different variants differ on how to compute $\boldsymbol{H}_{k+1}$
- Normally $\boldsymbol{H}_k^{-1}$ or its factorized version stored to simplify calculation of $\Delta \boldsymbol{x}_k$

Credit: UCLA ECE236C

BFGS method

Broyden–Fletcher–Goldfarb–Shanno (BFGS) method

BFGS update

$$H_{k+1} = H_k + \frac{yy^T}{y^T s} - \frac{H_k s s^T H_k}{s^T H_k s}$$

where

$$s = x_{k+1} - x_k, \qquad y = \nabla f(x_{k+1}) - \nabla f(x_k)$$

Inverse update

$$H_{k+1}^{-1} = \left(I - \frac{sy^T}{y^T s}\right) H_k^{-1} \left(I - \frac{ys^T}{y^T s}\right) + \frac{ss^T}{y^T s}$$

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Cost of update: $O(n^2)$ (vs. $O(n^3)$ in Newton's method), storage: $O(n^2)$ To derive the update equations, three conditions are imposed:

- secant condition: $\boldsymbol{H}_{k+1}\boldsymbol{s} = \boldsymbol{y}$ (think of 1st Taylor expansion to ∇f)
- Curvature condition: $\boldsymbol{s}_k^\mathsf{T}\boldsymbol{y}_k > 0$ to ensure that $\boldsymbol{H}_{k+1} \succ \mathbf{0}$ if $\boldsymbol{H}_k \succ \mathbf{0}$
- $\boldsymbol{H}_{k+1}$ and $\boldsymbol{H}_k$ are close in an appropriate sense

See Chap 6 of [Nocedal and Wright, 2006] Credit: UCLA ECE236C

Limited-memory BFGS (L-BFGS)

Limited-memory BFGS (L-BFGS): do not store H_k^{-1} explicitly

- instead we store up to m (*e.g.*, $m = 30$) values of

$$s_j = x_{j+1} - x_j, \qquad y_j = \nabla f(x_{j+1}) - \nabla f(x_j)$$

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Cost of update: $O(mn)$ (vs. $O(n^2)$ in BFGS), storage: $O(mn)$ (vs. $O(n^2)$ in BFGS) — linear in dimension n! recall the cost of GD?

See Chap 7 of [Nocedal and Wright, 2006] Credit: UCLA ECE236C

Outline

Block coordinate descent

Consider a function $f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_p)$ with $\boldsymbol{x}_1 \in \mathbb{R}^{n_1}$, ..., $\boldsymbol{x}_p \in \mathbb{R}^{n_p}$

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A generic block coordinate descent algorithm

Input: initialization $(\boldsymbol{x}_{1,0}, \ldots, \boldsymbol{x}_{p,0})$ (the 2nd subscript indexes iteration number)

1: **for** $k = 1, 2, \ldots$ **do**

2: Pick a block index $i \in \{1, \ldots, p\}$

3: Minimize wrt the chosen block:

$\boldsymbol{x}_{i,k} = \arg\min_{\boldsymbol{\xi} \in \mathbb{R}^{n_i}} \; f(\boldsymbol{x}_{1,k-1}, \ldots, \boldsymbol{x}_{i-1,k-1}, \boldsymbol{\xi}, \boldsymbol{x}_{i+1,k-1}, \ldots, \boldsymbol{x}_{p,k-1})$

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- In Line 2, many different ways of picking an index, e.g., cyclic, randomized, weighted sampling, etc

Block coordinate descent: examples

Least-squares $\min_{\boldsymbol{x}} \ f(\boldsymbol{x}) = \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2$

- $\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2 = \left\|\boldsymbol{y} - \boldsymbol{A}_{-i}\boldsymbol{x}_{-i} - \boldsymbol{a}_i x_i\right\|^2$
- coordinate descent: $\min_{\xi \in \mathbb{R}} \ \left\|\boldsymbol{y} - \boldsymbol{A}_{-i}\boldsymbol{x}_{-i} - \boldsymbol{a}_i \xi\right\|^2$

$$\Longrightarrow x_{i,+} = \frac{\langle \boldsymbol{y} - \boldsymbol{A}_{-i}\boldsymbol{x}_{-i}, \boldsymbol{a}_i \rangle}{\|\boldsymbol{a}_i\|_2^2}$$

($\boldsymbol{A}_{-i}$ is $\boldsymbol{A}$ with the i-th column removed; $\boldsymbol{x}_{-i}$ is $\boldsymbol{x}$ with the i-th coordinate removed)

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Matrix factorization $\min_{\boldsymbol{A},\boldsymbol{B}} \; \|\boldsymbol{Y} - \boldsymbol{A}\boldsymbol{B}\|_F^2$

- Two groups of variables, consider block coordinate descent
- Updates:

$$\boldsymbol{A}_+ = \boldsymbol{Y}\boldsymbol{B}^\dagger,$$
$$\boldsymbol{B}_+ = \boldsymbol{A}^\dagger \boldsymbol{Y}.$$

$(\cdot)^\dagger$ denotes the matrix pseudoinverse.)

Why block coordinate descent?

– may work with constrained problems and non-differentiable problems (e.g., $\min_{\boldsymbol{A},\boldsymbol{B}} \ \|\boldsymbol{Y} - \boldsymbol{A}\boldsymbol{B}\|_F^2, \ \mathrm{s.\,t.} \ \boldsymbol{A}$ orthogonal, Lasso: $\min_{\boldsymbol{x}} \ \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2 + \lambda \|\boldsymbol{x}\|_1$)

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Some references:

- [Wright, 2015]
- Lecture notes by Prof. Ruoyu Sun

Outline

Conjugate direction methods

Solve linear equation $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} \Longleftrightarrow \min_{\boldsymbol{x}} \ \frac{1}{2}\boldsymbol{x}^\intercal \boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}^\intercal \boldsymbol{x}$ with $\boldsymbol{A} \succ \boldsymbol{0}$

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apply coordinate descent...

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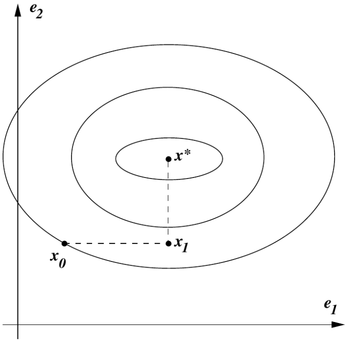
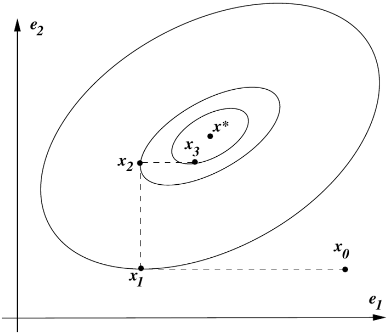


diagonal $\boldsymbol{A}$: solve the problem in n steps



non-diagonal $\boldsymbol{A}$: does not solve the problem in n steps

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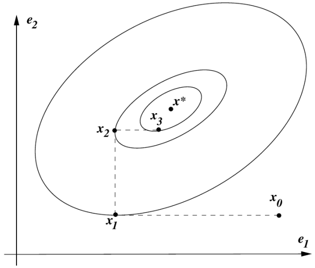

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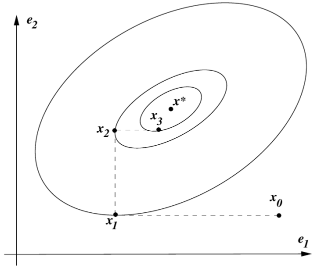

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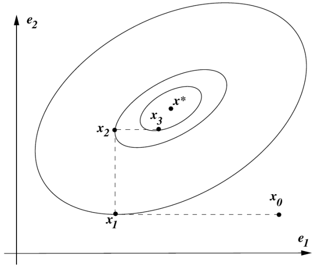

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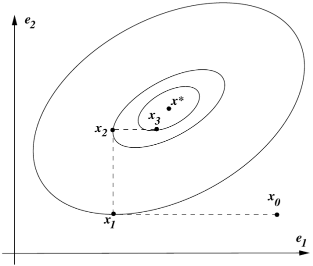

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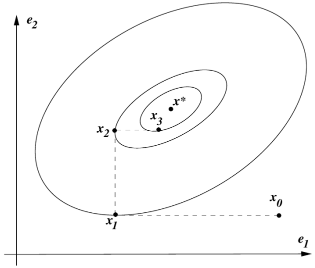

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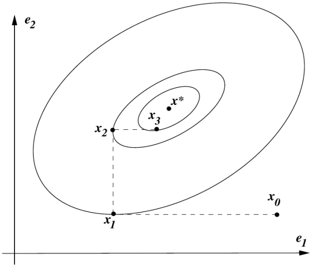

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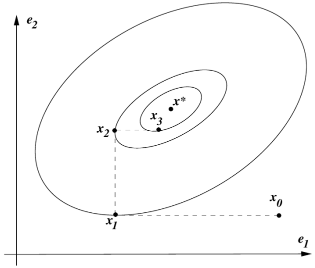

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In short, change of variable trick!

Conjugate gradient methods

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Idea: define n "conjugate directions" $\{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\}$ so that $\boldsymbol{p}_i^\intercal \boldsymbol{A}\boldsymbol{p}_j = 0$ for all $i \neq j$—conjugate as generalization of orthogonal

Generally, many choices for $\{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\}$.

Conjugate gradient methods: choice based on ideas from steepest descent

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Conjugate gradient methods: choice based on ideas from steepest descent

Algorithm 5.2 (CG).

Given x_0;

Set $r_0 \leftarrow Ax_0 - b$, $p_0 \leftarrow -r_0$, $k \leftarrow 0$;

while $r_k \neq 0$

$$\alpha_k \leftarrow \frac{r_k^T r_k}{p_k^T A p_k}; \tag{5.24a}$$

$$x_{k+1} \leftarrow x_k + \alpha_k p_k; \tag{5.24b}$$

$$r_{k+1} \leftarrow r_k + \alpha_k A p_k; \tag{5.24c}$$

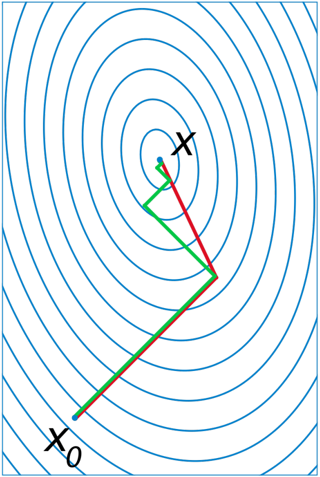
$$\beta_{k+1} \leftarrow \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k}; \tag{5.24d}$$

$$p_{k+1} \leftarrow -r_{k+1} + \beta_{k+1} p_k; \tag{5.24e}$$

$$k \leftarrow k + 1; \tag{5.24f}$$

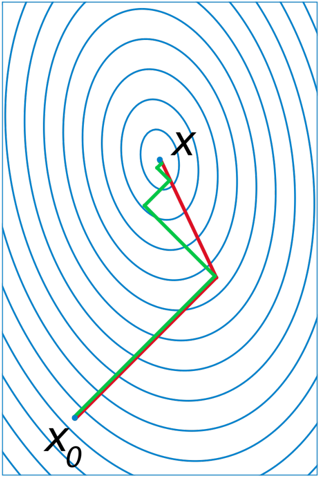
end (while)

Conjugate gradient methods



CG vs. GD (Green: GD, Red: CG)

Conjugate gradient methods



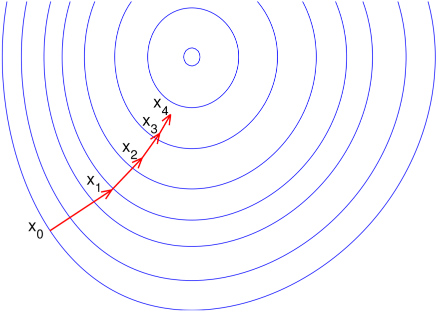
CG vs. GD (Green: GD, Red: CG)

- Can be extended to general non-quadratic functions
- Often used to solve subproblems of other iterative methods, e.g., truncated Newton method, the trust-region subproblem (later)

See Chap 5 of [Nocedal and Wright, 2006]

Outline

Iterative methods



Credit: aria42.com

Illustration of iterative methods on the contour/levelset plot (i.e., the function assumes the same value on each curve)

Two questions: what direction to move, and how far to move

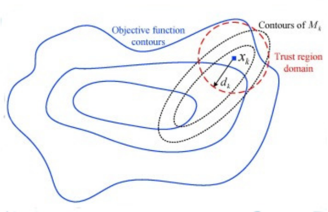
Two possibilities:

- **Line-search methods**: direction first, size second
- **Trust-region methods** (TRM): size first, direction second

Ideas behind TRM

Recall Taylor expansion $f(\boldsymbol{x}+\boldsymbol{d}) \approx f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{d} \rangle + \frac{1}{2} \langle \boldsymbol{d}, \nabla^2 f(\boldsymbol{x}_k) \boldsymbol{d} \rangle$

Start with $\boldsymbol{x}_0$. Repeat the following:



Credit: [Arezki et al., 2018]

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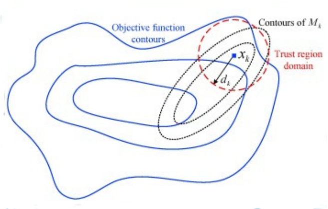

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Start with $\boldsymbol{x}_0$. Repeat the following:

– At $\boldsymbol{x}_k$, approximate f by the quadratic function (called model function dotted black)

$$m_k(\boldsymbol{d}) = f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{d}\rangle + \frac{1}{2}\langle \boldsymbol{d}, \boldsymbol{B}_k \boldsymbol{d}\rangle$$

i.e., $m_k(\boldsymbol{d}) \approx f(\boldsymbol{x}_k + \boldsymbol{d})$, and $\boldsymbol{B}_k$ to approximate $\nabla^2 f(\boldsymbol{x}_k)$

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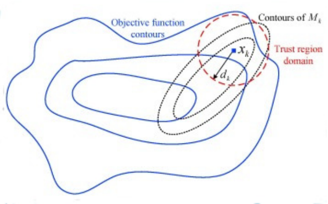

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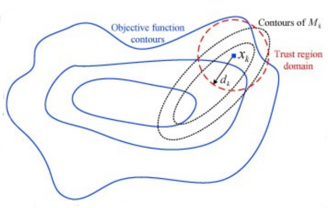

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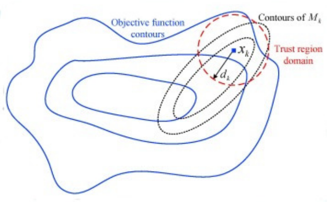

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- If the approximation is inaccurate, decrease the region size; if the approximation is sufficiently accurate, increase the region size.
- If the approximation is reasonably accurate, update the iterate $\boldsymbol{x}_{k+1} = x_k + \boldsymbol{d}_k$.

Framework of trust-region methods

To measure approximation quality: $\rho_k \doteq \frac{f(\boldsymbol{x}_k)-f(\boldsymbol{x}_k+\boldsymbol{d}_k)}{m_k(\mathbf{0})-m_k(\boldsymbol{d}_k)} = \frac{\text{actual decrease}}{\text{model decrease}}$

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A generic trust-region algorithm

Input: $\boldsymbol{x}_0$, radius cap $\widehat{\Delta} > 0$, initial radius Δ_0, acceptance ratio $\eta \in [0, 1/4)$

for $k = 0, 1, \ldots$ **do**
    $\boldsymbol{d}_k = \arg\min_{\boldsymbol{d}} m_k(\boldsymbol{d})\,, \ \text{s.t.}\ \|\boldsymbol{d}\| \le \Delta_k$ **(TR Subproblem)**
    if $\rho_k < 1/4$ **then**
        $\Delta_{k+1} = \Delta_k/4$
    else
        if $\rho_k > 3/4$ and $\|\boldsymbol{d}_k\| = \Delta_k$ **then**
            $\Delta_{k+1} = \min\left(2\Delta_k, \widehat{\Delta}\right)$
        else
            $\Delta_{k+1} = \Delta_k$
        end if
    end if
    if $\rho_k > \eta$ **then**
        $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{d}_k$
    else
        $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k$
    end if
end for

Why TRM?

Recall the model function $m_k(\boldsymbol{d}) \doteq f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{d} \rangle + \frac{1}{2} \langle \boldsymbol{d}, \boldsymbol{B}_k \boldsymbol{d} \rangle$

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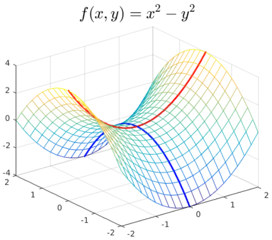

When $\nabla f(\boldsymbol{x}_k) = \mathbf{0}$,

$$m_k(\boldsymbol{d}) - f(\boldsymbol{x}_k) = \frac{1}{2} \left\langle \boldsymbol{d}, \nabla^2 f(\boldsymbol{x}_k)\, \boldsymbol{d} \right\rangle .$$

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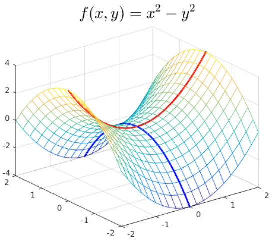

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If $\nabla^2 f(\boldsymbol{x}_k)$ has negative eigenvalues, i.e., there are negative directional curvatures, $\frac{1}{2} \left\langle \boldsymbol{d}, \nabla^2 f(\boldsymbol{x}_k)\, \boldsymbol{d} \right\rangle < 0$ for certain choices of $\boldsymbol{d}$ (e.g., eigenvectors corresponding to the negative eigenvalues)

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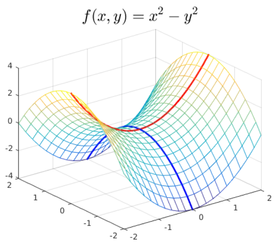

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TRM can help to move away from "nice" saddle points!

To learn more about TRM

- A comprehensive reference [Conn et al., 2000]
- A closely-related alternative: cubic regularized second-order (CRSOM)
  method [Nesterov and Polyak, 2006, Agarwal et al., 2018]
- Example implementation of both TRM and CRSOM: Manopt (in Matlab) `https://www.manopt.org/` (choosing the Euclidean manifold)

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