Optimization for Datascience

Convexity, Smoothness and the Gradient Method

Robert M. Gower

TELECOM ParisTech

Today we will

- **Lecture:** Basic theory and exercises on convexity, smoothness, strong convexity and convergence proofs
- **Exercises lists:**

  complexity_rates_exe

  exe_convexity_smoothness

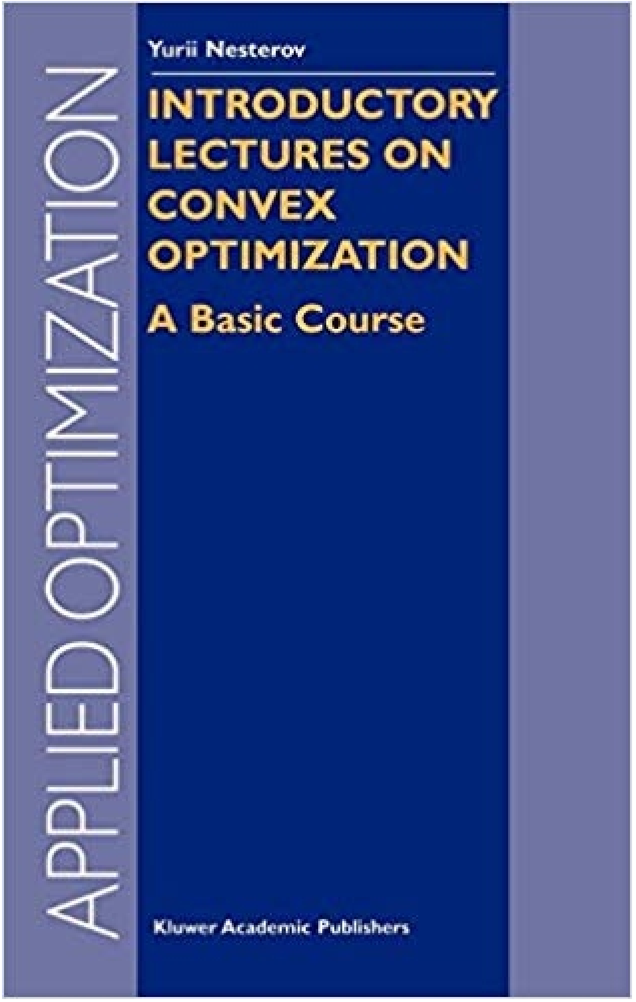
  ridge_reg_exe

References for todays class

Yurii Nestorov (2004)
Introductory Lectures on Convex Programming

Chapter 1 and Section 2.1

Free pdf online !



Solving the Finite Sum Training Problem

Optimization Sum of Terms

A Datum Function

$$f_i(w) := \ell\left(h_w(x^i), y^i\right) + \lambda R(w)$$

$$\begin{aligned}
\frac{1}{n}\sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right) + \lambda R(w) &= \frac{1}{n}\sum_{i=1}^{n} \left(\ell\left(h_w(x^i), y^i\right) + \lambda R(w)\right) \\
&= \frac{1}{n}\sum_{i=1}^{n} f_i(w)
\end{aligned}$$

Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n}\sum_{i=1}^{n} f_i(w) =: f(w)$$

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Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n}\sum_{i=1}^{n} f_i(w) =: f(w)$$

How to solve unconstrained optimization?

The Training Problem

Solving the *training problem*: $$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w)$$

Reference method: Gradient descent

$$\nabla \left(\frac{1}{n} \sum_{i=1}^{n} f_i(w) \right) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(w)$$

Gradient Descent Algorithm

Set $w^0 = 0$, choose $\alpha > 0$.

for $t = 1, 2, 3, \ldots, T$

$$w^{t+1} = w^t - \frac{\alpha}{n} \sum_{i=1}^{n} \nabla f_i(w^t)$$

Output w^{T+1}

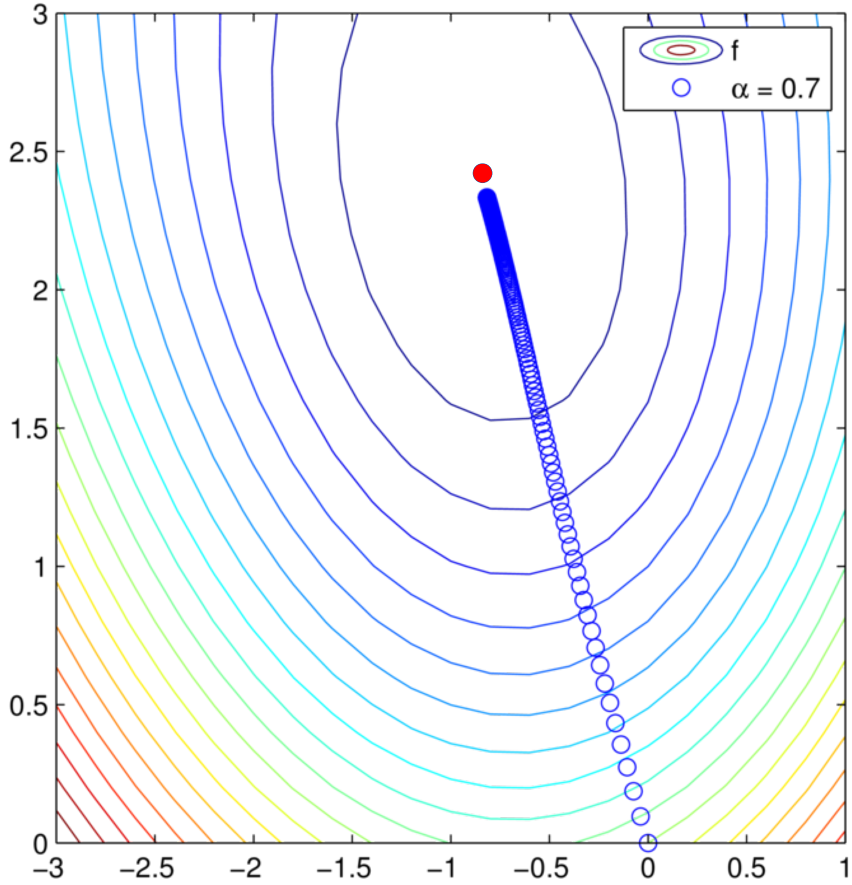
Gradient Descent Example

A Logistic Regression problem using the fourclass labelled data from LIBSVM

$(n,\ d)=(862{,}2)$

Logistic Regression

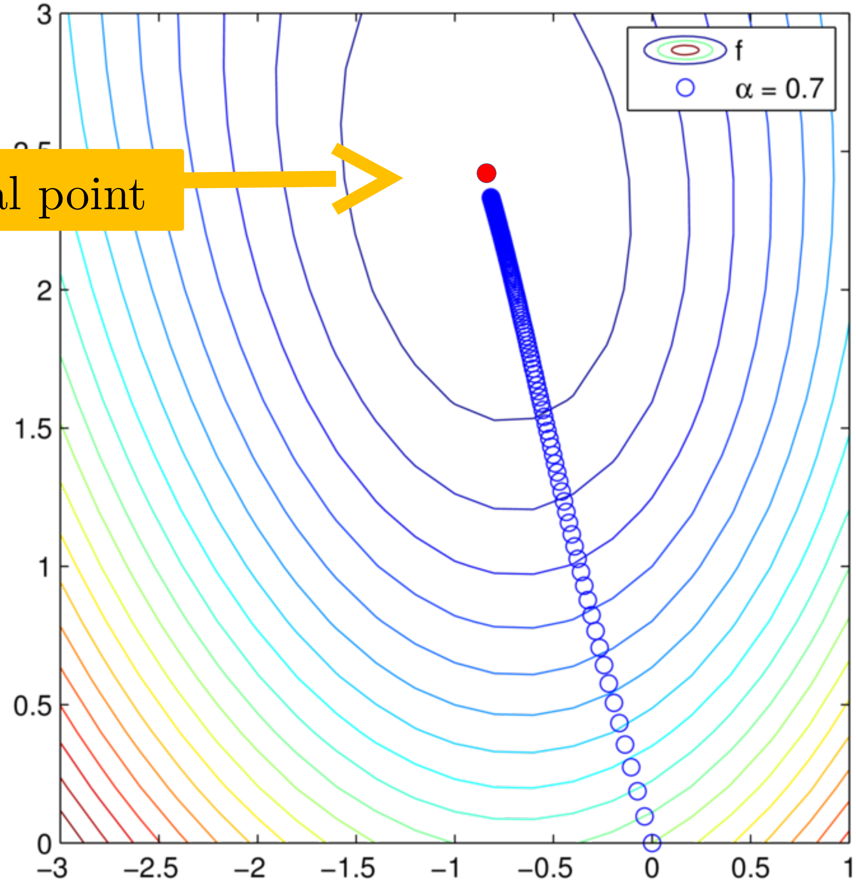
$$\min_{w\in\mathbf{R}^d} \frac{1}{n}\sum_{i=1}^{n}\ln(1+e^{-y^i\langle w,x^i\rangle})+\lambda||w||_2^2$$



Can we prove that this always works?

Gradient Descent Example

Optimal point



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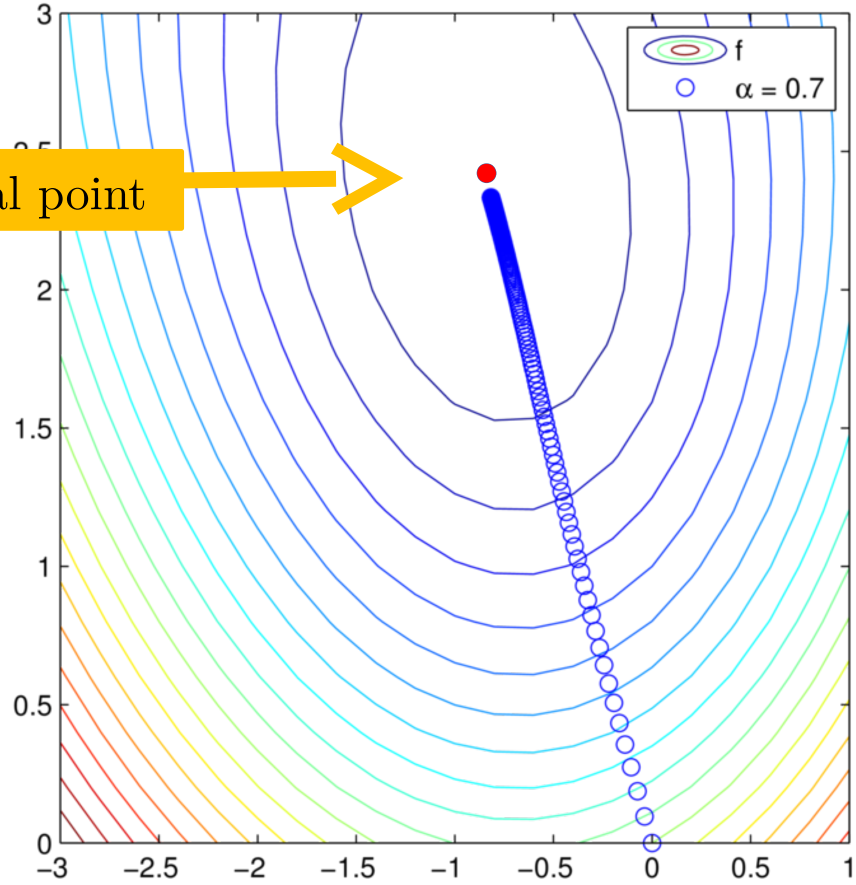

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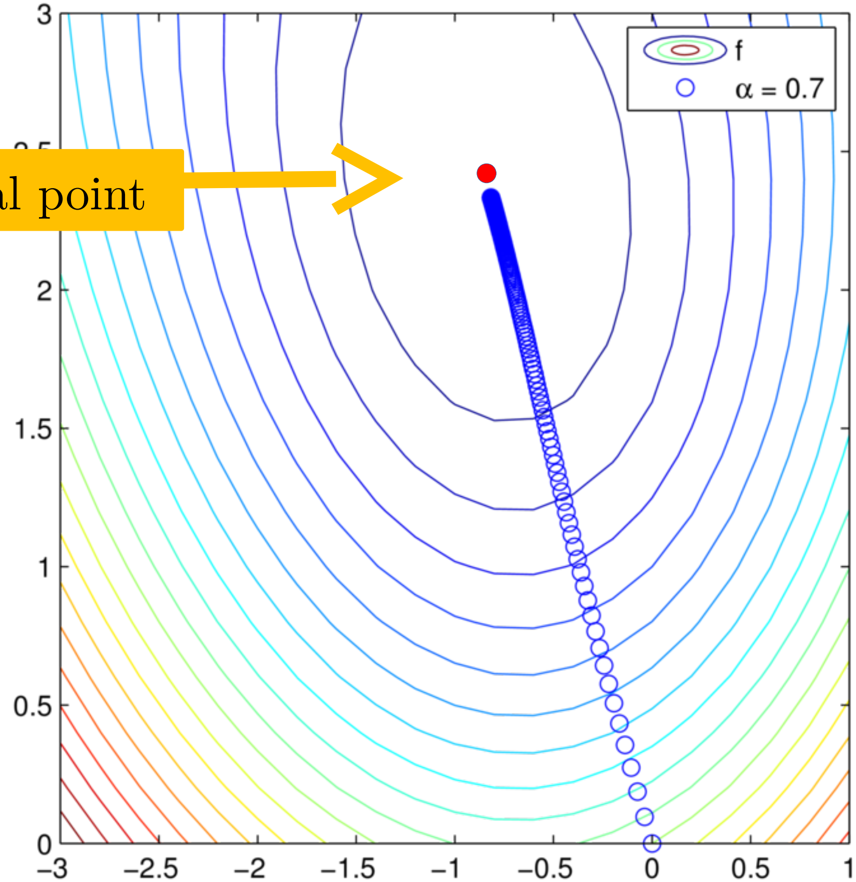
Can we prove that this always works?

No! There is no universal optimization method. The "no free lunch" of Optimization

Gradient Descent Example

Optimal point



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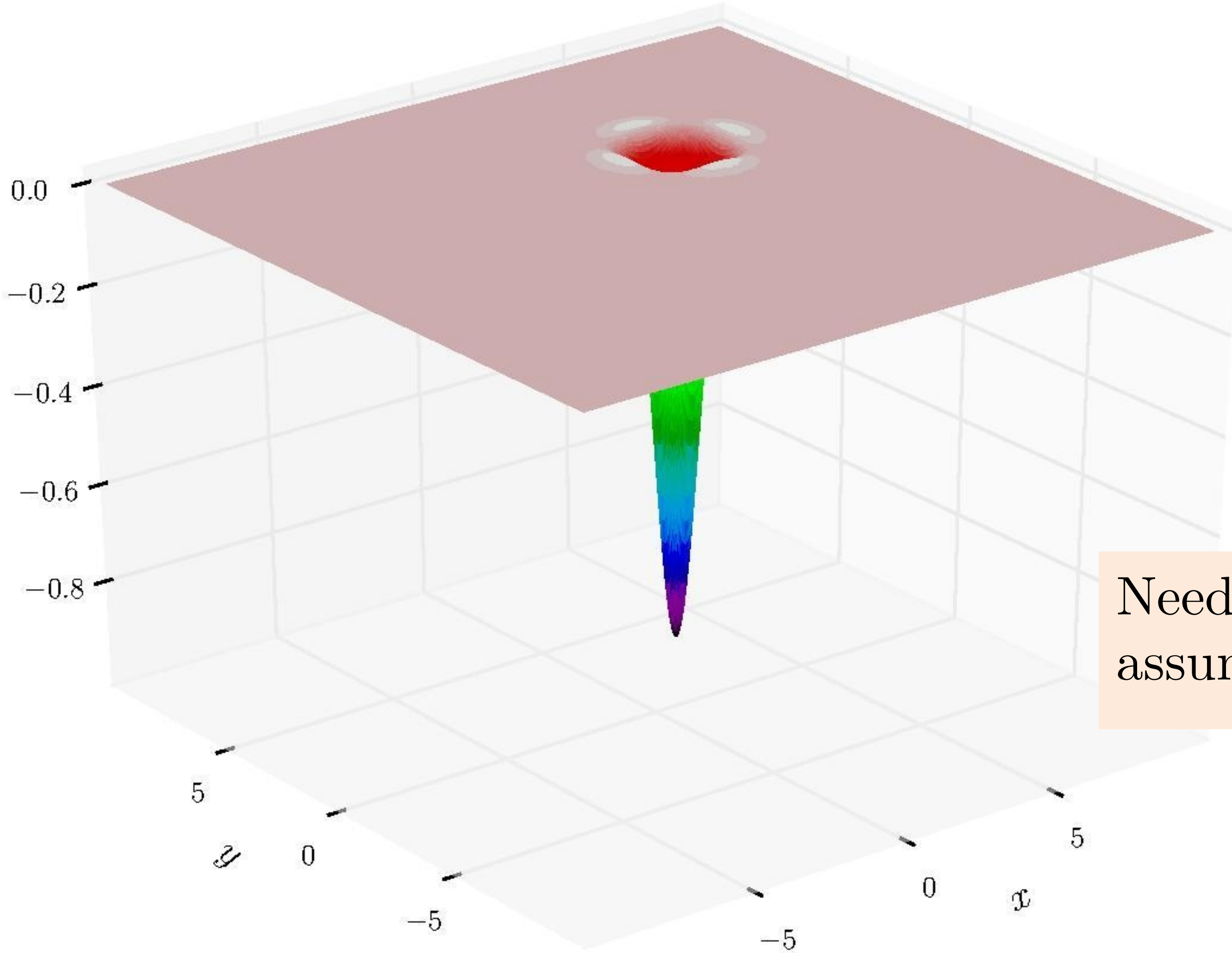
Specialize

Convex and smooth training problems

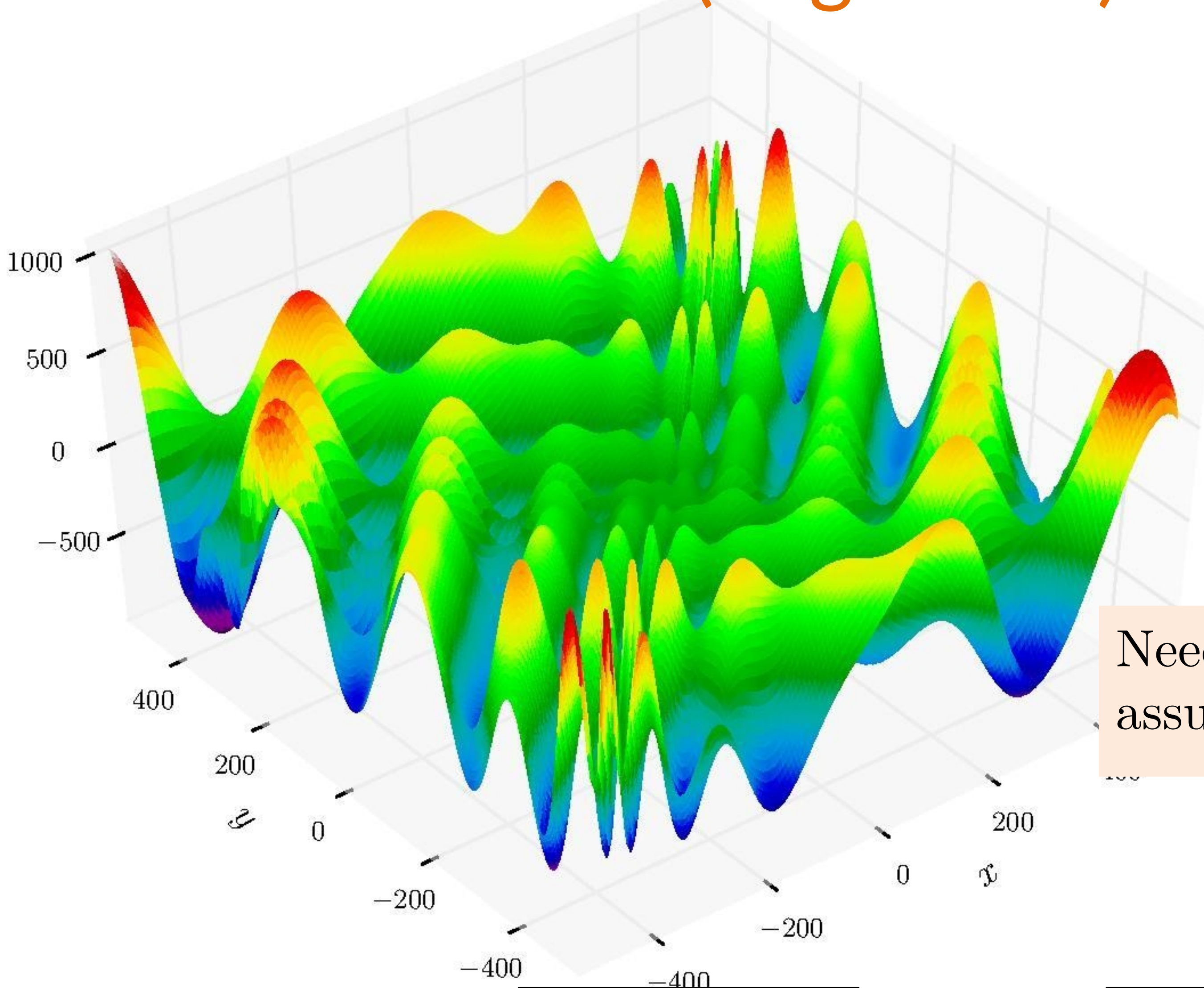
Optimization is hard (in general)



Need assumptions!

$$f(x, y) = -\cos(x)\cos(y)\exp\left(-(x-\pi)^2 - (y-\pi)^2\right)$$

Optimization is hard (in general)

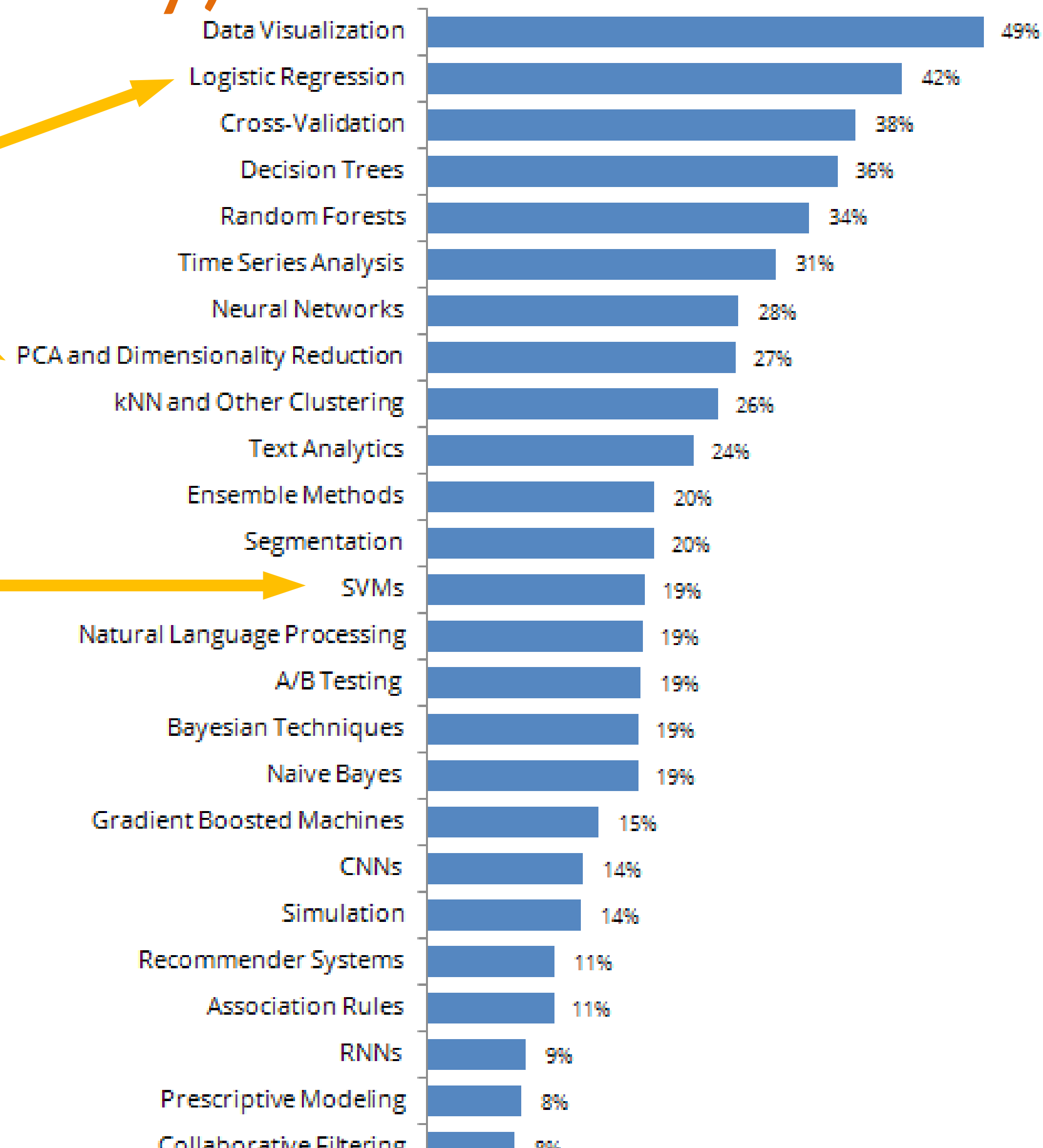


Need assumptions!

$$f(x,y) = -(y+47)\sin\sqrt{\left|\frac{x}{2}+(y+47)\right|} - x\sin\sqrt{\left|\frac{x}{2}-(y+47)\right|}$$

Data science methods most used (Kaggle 2017 survey)

Convex Optimization problems



Main assumption

Nice property

$$\text{If } \nabla f(w^*) = 0 \quad \text{then} \quad f(w^*) \leq f(w), \quad \forall w \in \mathbb{R}^d$$

All stationary points are global minima

Lemma: Convexity => Nice property

$$\text{If } \; f(w) \geq f(y) + \langle \nabla f(y), w - y \rangle, \quad \forall w, y \in \mathbb{R}^d$$

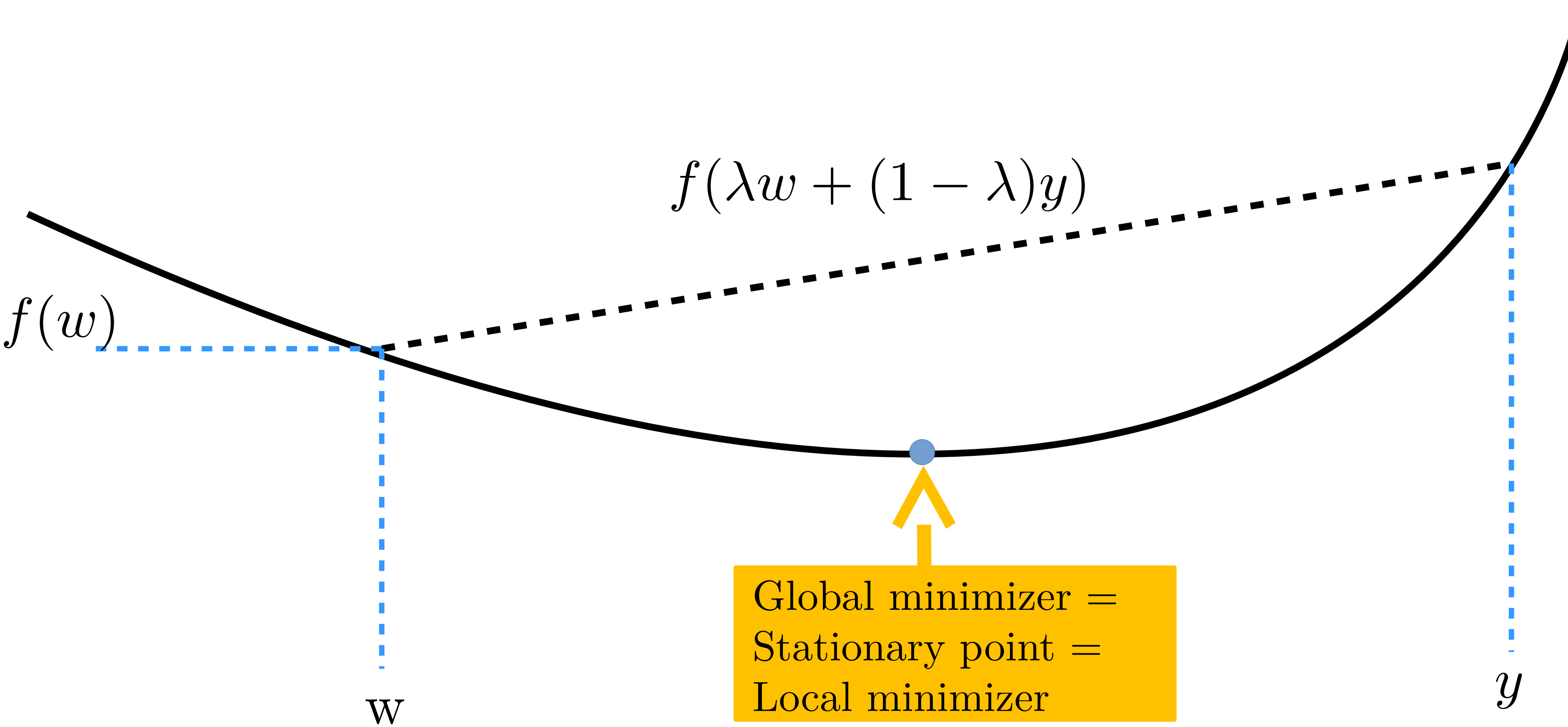
then nice property holds

PROOF: Choose $y = w^*$

Convexity

We say $f : \mathrm{dom}(f) \subset \mathbb{R}^n \to \mathbb{R}$ is convex if $\mathrm{dom}(f)$ is convex and

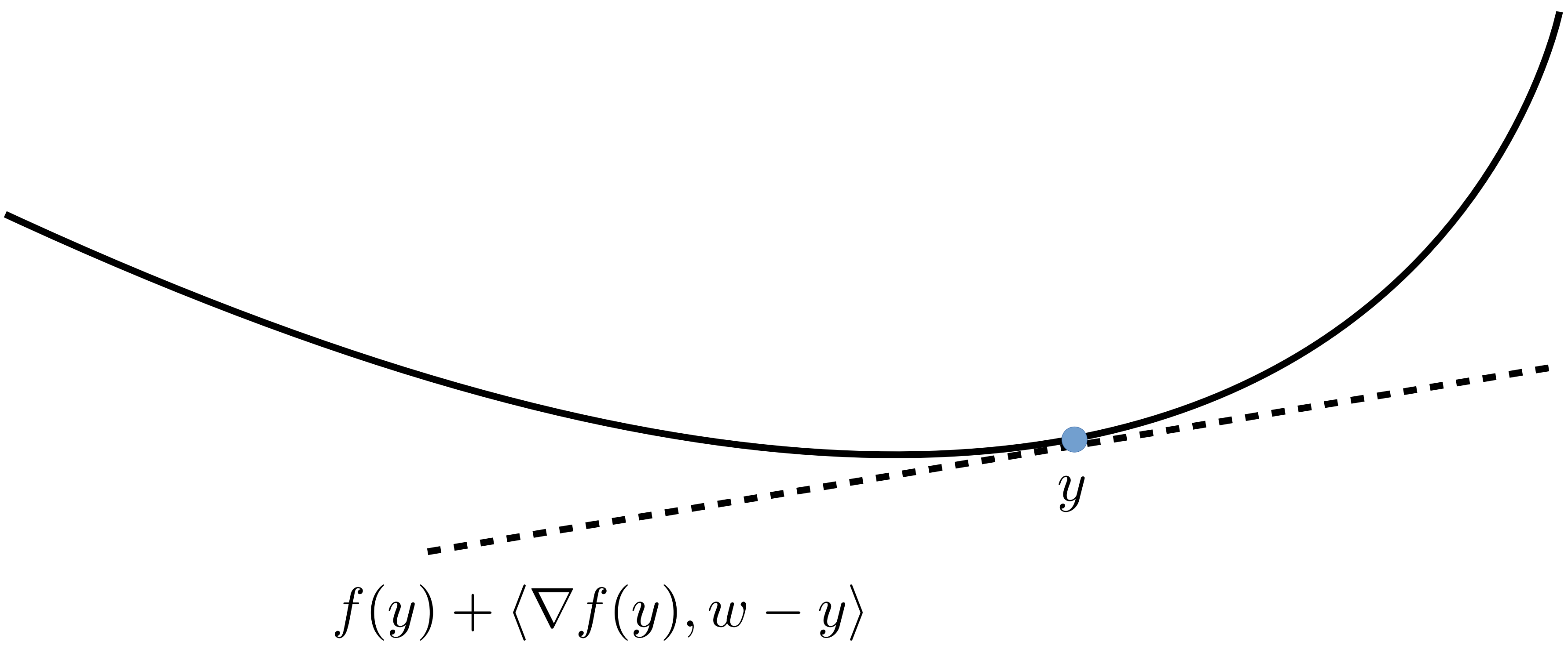
$$f(\lambda w + (1-\lambda)y) \leq \lambda f(w) + (1-\lambda) f(y), \quad \forall w, y \in C, \lambda \in [0, 1]$$



Convexity: First derivative

A differential function $f : \mathrm{dom}(f) \subset \mathbb{R}^n \to \mathbb{R}$ is convex iff

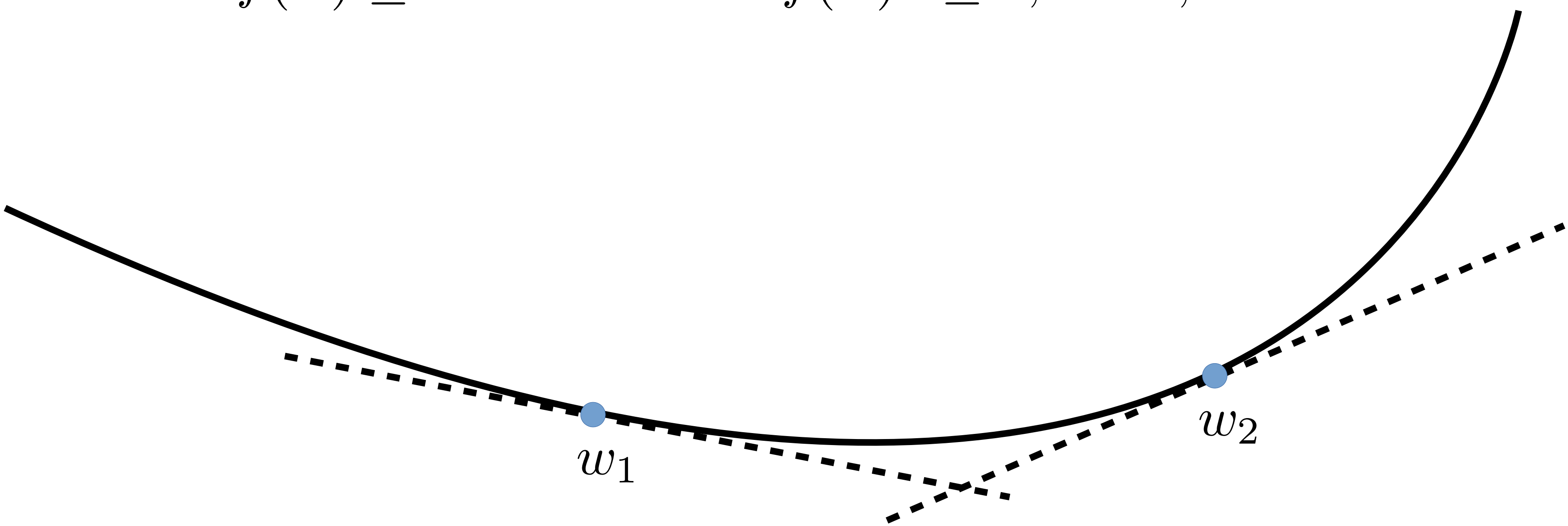
$$f(w) \geq f(y) + \langle \nabla f(y), w - y \rangle$$



Convexity: Second derivative

A twice differential function $f : \mathrm{dom}(f) \subset \mathbb{R}^n \to \mathbb{R}$ is convex iff

$$\nabla^2 f(w) \succeq 0 \quad \Leftrightarrow \quad v^\top \nabla^2 f(w) v \geq 0, \quad \forall w, v \in \mathbb{R}^n$$



$$w_1 \leq w_2 \quad \Rightarrow f'(w_1) \leq f'(w_2)$$

Convexity: Examples

Extended-value extension:

$$f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$$

$$f(x) = \infty, \quad \forall x \notin \mathrm{dom}(f)$$

Norms and squared norms:

$$x \mapsto ||x||$$

$$x \mapsto ||x||^2$$

Proof is an exercise!

Negative log and logistic:

$$x \mapsto -\log(x)$$

$$x \mapsto \log\left(1 + e^{-y\langle a,x\rangle}\right)$$

Hinge loss

$$x \mapsto \max\{0, 1 - yx\}$$

Negatives log determinant, exponentiation ... etc

Smoothness

We say $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is smooth if

$$||\nabla f(x) - \nabla f(y)|| \leq L||x - y||, \quad \forall x, y \in \mathbb{R}^n$$

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If a twice differentiable $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is L–smooth then

1) $$d^\top \nabla^2 f(x) d \leq L \cdot ||d||_2^2, \quad \forall x, d \in \mathbb{R}^n$$

2) $$f(x) \leq f(y) + \langle \nabla f(y), x - y \rangle + \frac{L}{2}||x - y||^2, \quad \forall x, y \in \mathbb{R}^n$$

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EXE: Using that $$\sigma_{\max}(X)^2||d||_2^2 \geq ||X^\top d||_2^2$$

Show that $\frac{1}{2}||X^\top w - b||_2^2$ is $\sigma_{\max}(X)^2$–smooth

Smoothness: Examples

Convex quadratics: $x \mapsto x^\top A x + b^\top x + c$

Logistic: $x \mapsto \log\left(1 + e^{-y\langle a, x\rangle}\right)$

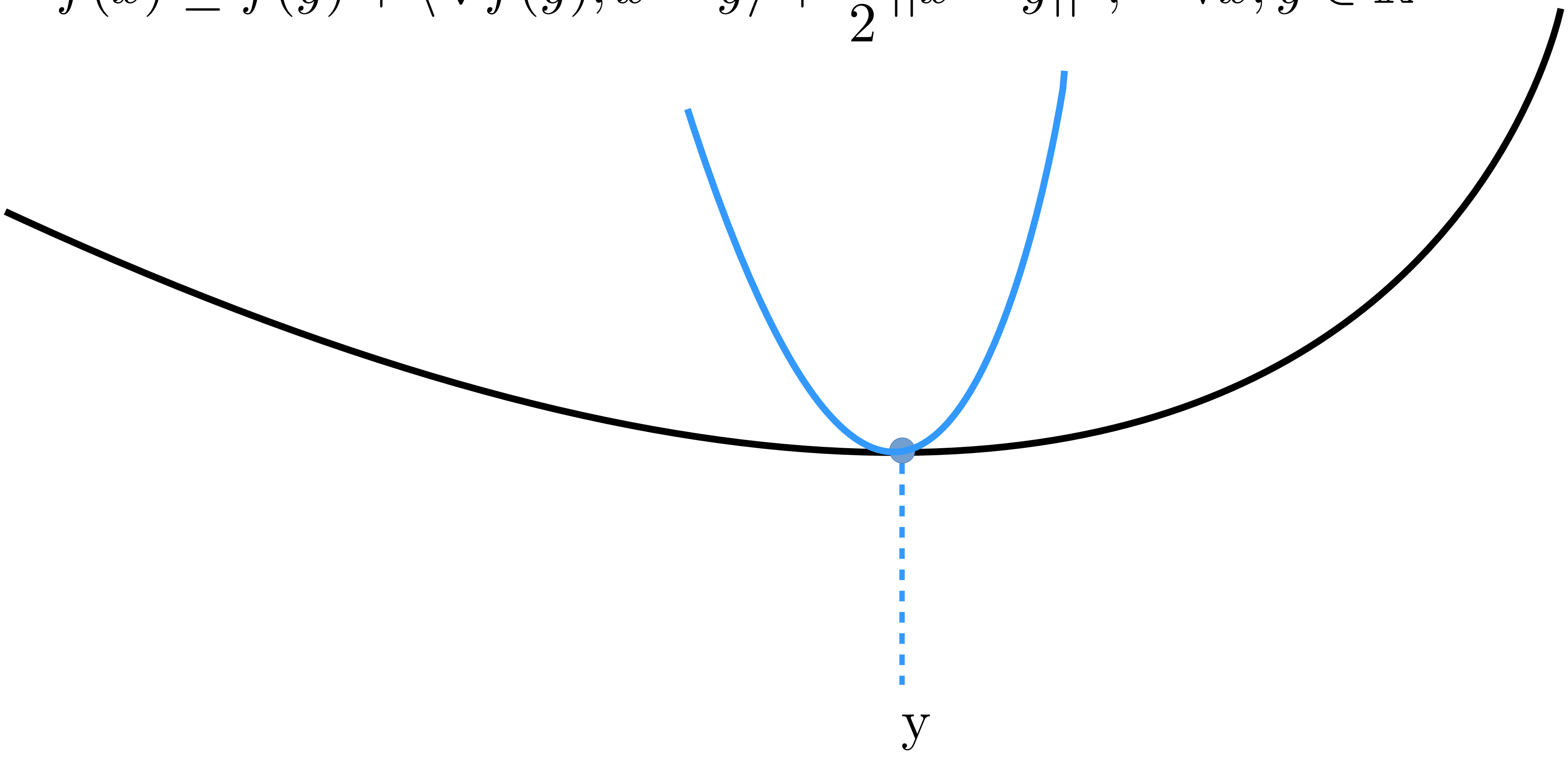
Trigonometric: $x \mapsto \cos(x), \sin(x)$

Proof is an exercise!

Important consequences of Smoothness

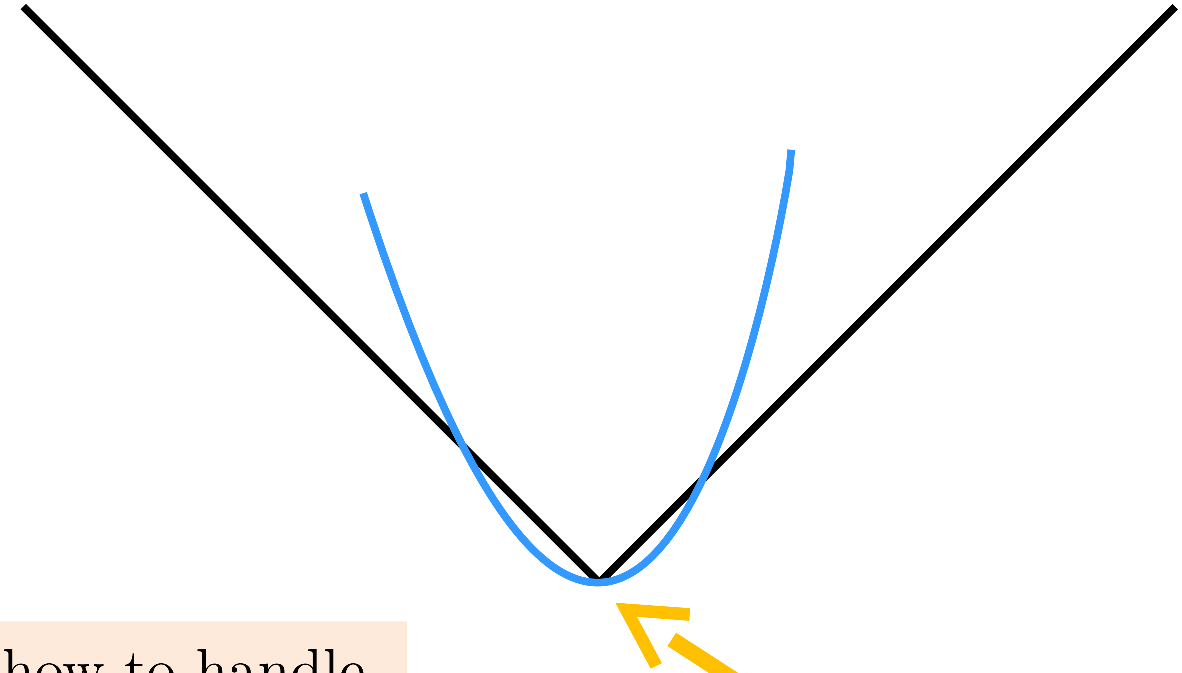
If $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is L–smooth then

$$f(x) \leq f(y) + \langle \nabla f(y), x - y \rangle + \frac{L}{2}||x - y||^2, \quad \forall x, y \in \mathbb{R}^n$$



Smoothness: Convex counter-example

$$f(w) = ||w||_1 = \sum_{i=1}^{n} |w_i|$$



We'll see how to handle this problem next class

Does not fit.
Not smooth

Insight into Gradient Descent

$$\boxed{f(w) \leq f(y) + \langle \nabla f(y), w - y \rangle + \frac{L}{2}||w - y||^2, \quad \forall w, y \in \mathbb{R}^n}$$

Minimizing the upper bound in w we get:

$$\nabla_w \left(f(y) + \langle \nabla f(y), w - y \rangle + \frac{L}{2}||w - y||^2 \right) = \nabla f(y) + L(w - y) = 0$$

Insight into Gradient Descent

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$$\Downarrow$$

$$w = y - \frac{1}{L} \nabla f(y)$$

Insight into Gradient Descent

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A gradient descent step !

$$w = y - \frac{1}{L}\nabla f(y)$$

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$$\nabla_w \left(f(y) + \langle \nabla f(y), w - y \rangle + \frac{L}{2}||w-y||^2 \right) = \nabla f(y) + L(w-y) = 0$$

EXE: **If f is L-smooth, show that**

$$f(y - \tfrac{1}{L}\nabla f(y)) - f(y) \leq -\frac{1}{2L}||\nabla f(y)||_2^2, \ \forall y$$

$$f(w^*) - f(w) \leq -\frac{1}{2L}||\nabla f(w)||_2^2, \quad \forall w \in \mathbb{R}^n$$

where $f(w^*) \leq f(w), \quad \forall w \in \mathbb{R}^n$

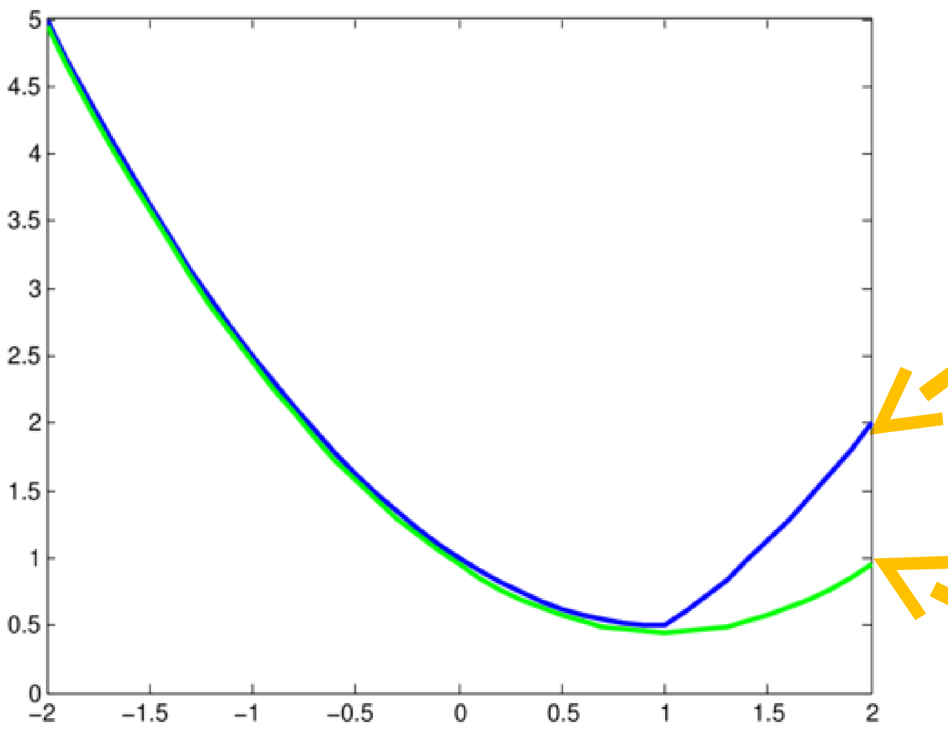
A gradient descent step !

$$w = y - \frac{1}{L}\nabla f(y)$$

Strong convexity

We say $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is μ–strongly convex if

$$\boxed{f(w) \geq f(y) + \langle \nabla f(y), w - y \rangle + \frac{\mu}{2}||w - y||^2, \quad \forall w, y \in \mathbb{R}^n}$$



Hinge loss + L2

$$\max\{0, 1 - w\} + \frac{1}{2}||w||_2^2$$

Quadratic lower bound

Strong convexity

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$$d^\top \nabla^2 f(w) d \geq \mu ||d||^2, \quad \forall d \in \mathbb{R}^n$$

EXE: Using that

$$\sigma_{\min}(X)^2 ||d||_2^2 \leq ||X^\top d||_2^2$$

Show that

$$\tfrac{1}{2}||X^\top w - b||_2^2 \text{ is } \sigma_{\min}(X)^2\text{–strongly convex}$$

Convergence GD strongly convex

Theorem

Let f be μ-strongly convex and L-smooth.

$$||w^t - w^*||_2^2 \leq \left(1 - \frac{\mu}{L}\right)^t ||w^1 - w^*||_2^2$$

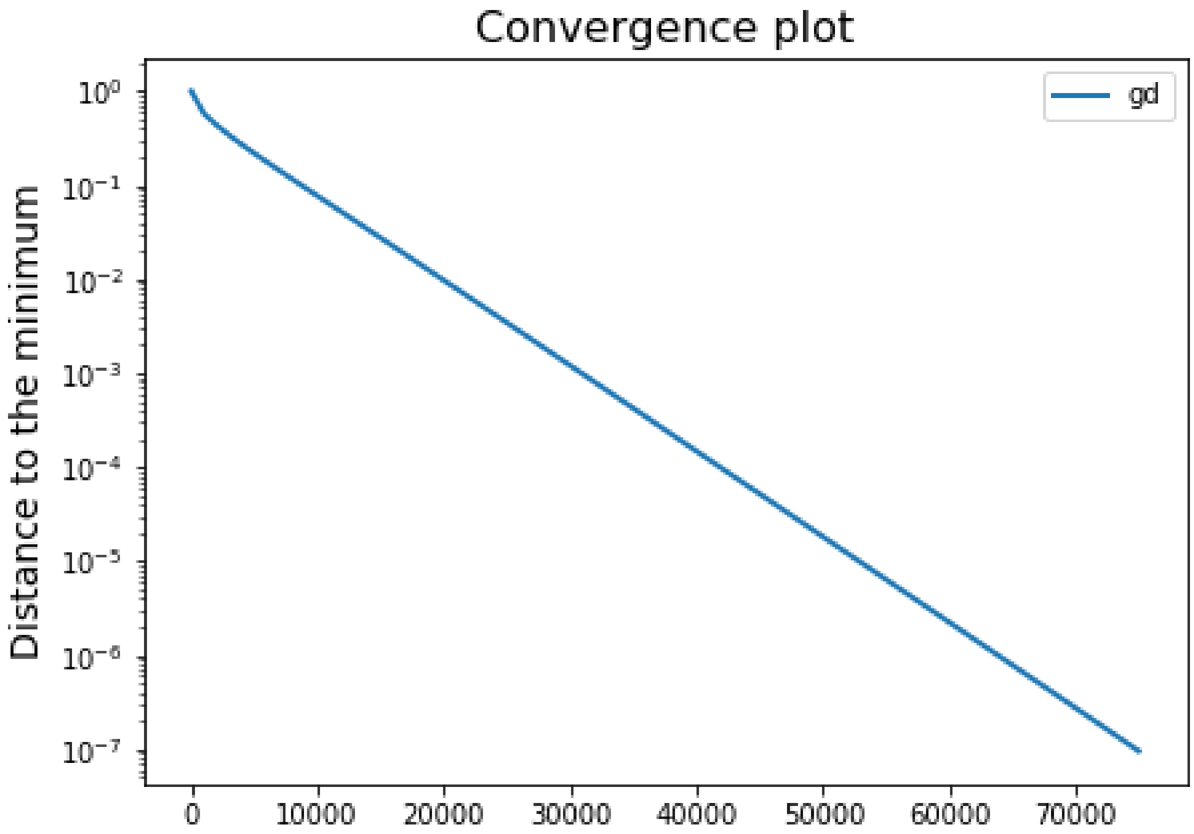
Where

$$w^{t+1} = w^t - \frac{1}{L}\nabla f(w^t), \quad \text{for } t = 1, \ldots, T$$

$$\Rightarrow \text{for } \frac{||w^T - w^*||_2^2}{||w^1 - w^*||_2^2} \leq \epsilon \text{ we need } T \geq \frac{L}{\mu}\log\left(\frac{1}{\epsilon}\right) = O\left(\log\left(\frac{1}{\epsilon}\right)\right)$$

EXE: Solve the questions in complexity_rates_exe.pdf

Gradient Descent Example: logistic



$$y\text{–axis} = \frac{||w^t - w^*||_2^2}{||w^1 - w^*||_2^2} \quad \Rightarrow \quad \log\left(\frac{||w^t - w^*||_2^2}{||w^1 - w^*||_2^2}\right) \leq t \log\left(1 - \frac{\mu}{L}\right)$$

Proof Convergence GD strongly convex + smooth

Proof on board

$$||w^{t+1} - w^*||_2^2 = ||w^t - w^* - \frac{1}{L}\nabla f(w^t)||_2^2$$

$$= ||w^t - w^*||_2^2 + \frac{2}{L}\langle \nabla f(w^t), w^* - w^t\rangle + \frac{1}{L^2}||\nabla f(w^t)||_2^2$$

Now smoothness gives

$$f(w^*) - f(w) \leq -\frac{1}{2L}||\nabla f(w)||_2^2$$

$$\Downarrow$$

$$||\nabla f(w)||_2^2 \leq 2L(f(w) - f(w^*))$$

And strong convexity gives

$$f(w^*) \geq f(w) + \langle \nabla f(w), w^* - w\rangle + \frac{\mu}{2}||w - w^*||^2$$

$$\Downarrow$$

$$\langle \nabla f(w), w^* - w\rangle \leq -(f(w) - f(w^*)) - \frac{\mu}{2}||w - w^*||^2$$

Convergence GD for smooth + convex

Theorem

Let f be convex and L-smooth.

$$f(w^t) - f(w^*) \le \frac{2L||w^1 - w^*||_2^2}{t-1} = O\left(\frac{1}{t}\right).$$

Where

$$w^{t+1} = w^t - \frac{1}{L}\nabla f(w^t)$$

$\Rightarrow$ for $\dfrac{f(w^T) - f(w^*)}{||w^1 - w^*||_2^2} \le \epsilon$ we need $T \ge \dfrac{2L}{\epsilon} = O\left(\dfrac{1}{\epsilon}\right)$

Convex and Smooth Properties

If $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ convex and L–smooth then

$$f(y) - f(x) \leq \langle \nabla f(y), y - x \rangle - \frac{1}{2L} ||\nabla f(y) - \nabla f(x)||_2^2$$

Co-coercivity

$$\langle \nabla f(y) - \nabla f(x), y - x \rangle \geq \frac{1}{L} ||\nabla f(x) - \nabla f(y)||_2$$

Proof

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Co-coercivity

$$\langle \nabla f(y) - \nabla f(x), y - x \rangle \geq \frac{1}{L} ||\nabla f(x) - \nabla f(y)||_2$$

Proof

$$f(y) - f(x) = \overbrace{f(y) - f(z)}^{\text{Use convexity}} + \overbrace{f(z) - f(x)}^{\text{Use smoothness}}$$

Convex and Smooth Properties

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Proof

$$f(y) - f(x) = \overbrace{f(y) - f(z)}^{\text{Use convexity}} + \overbrace{f(z) - f(x)}^{\text{Use smoothness}}$$

$$\leq \langle \nabla f(y), y - z \rangle + \langle \nabla f(x), z - x \rangle + \frac{L}{2} ||z - x||^2$$

Convex and Smooth Properties

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Co-coercivity

$$\langle \nabla f(y) - \nabla f(x), y - x \rangle \geq \frac{1}{L} ||\nabla f(x) - \nabla f(y)||_2$$

Proof

$$\begin{aligned} f(y) - f(x) &= \overbrace{f(y) - f(z)}^{\text{Use convexity}} + \overbrace{f(z) - f(x)}^{\text{Use smoothness}} \\ &\leq \langle \nabla f(y), y - z \rangle + \langle \nabla f(x), z - x \rangle + \frac{L}{2} ||z - x||^2 \end{aligned}$$

Then minimize in z and insert back in minima.

Proof of GD smooth + convex theorem

$$||w^{t+1} - w^*||_2^2 = ||w^t - w^* - \frac{1}{L}\nabla f(w^t)||_2^2$$

Use co-coercivity

$$= ||w^t - w^*||_2^2 + \frac{2}{L}\overbrace{\langle \nabla f(w^t), w^* - w^t\rangle} + \frac{1}{L^2}||\nabla f(w^t)||_2^2$$

Co-coercivity

$$\langle \nabla f(y) - \nabla f(w), y - w\rangle \geq \frac{1}{L}||\nabla f(w) - \nabla f(y)||_2$$

With $y = w^*$ gives $\quad \langle \nabla f(w), w^* - w\rangle \leq -\frac{1}{L}||\nabla f(w)||_2$

Inserting above show decreasing

$$||w^{t+1} - w^*||_2^2 \leq ||w^t - w^*||_2^2 - \frac{1}{L^2}||\nabla f(w^t)||_2^2$$

smoothness gives

$$f(w^{t+1}) - f^* \leq f(w^t) - f^* - \frac{1}{2L}||\nabla f(w^t)||_2^2$$

Combine with convexity

$$\begin{aligned} f(w^t) - f(w^*) &\leq \langle \nabla f(w^t), w^t - w^*\rangle \\ &\leq ||\nabla f(w^t)||_2 ||w^t - w^*||_2 \end{aligned}$$

Acceleration and lower bouds

The Accelerated gradient method

$$\min_{w \in \mathbb{R}^d} f(w)$$

Accelerated gradient

Set $w^1 = 0 = y^1, \kappa = L/\mu$

for $t = 1, 2, 3, \ldots, T$

$$y^{t+1} = w^t - \frac{1}{L}\nabla f(w^t)$$

$$w^{t+1} = \left(1 + \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right) y^{t+1} - \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} w^t$$

Output w^{T+1}

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$$\min_{w \in \mathbb{R}^d} f(w)$$

Accelerated gradient

Set $w^1 = 0 = y^1, \kappa = L/\mu$

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$$y^{t+1} = w^t - \frac{1}{L}\nabla f(w^t)$$

$$w^{t+1} = \left(1 + \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right) y^{t+1} - \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} w^t$$

Output w^{T+1}

Weird extrapolation, but it works

Convergence lower bounds strongly convex

Theorem (Nesterov)

For any optimization algorithm where

$$w^{t+1} \in w^t + \mathrm{span}\left(\nabla f(w^1), \nabla f(w^2), \ldots, \nabla f(w^t)\right)$$

There exists a function $f(w)$ that is L–smooth and μ–strongly convex such that

$$f(w^T) - f(w^*) \geq \frac{\mu}{2}\left(1 - \frac{2}{\sqrt{\kappa + 1}}\right)^{2(T-1)} ||w^1 - w^*||_2^2$$

$$= O\left(\left(1 - \frac{1}{\sqrt{\kappa}}\right)^{2T}\right).$$

Accelerated gradient has this rate

Yuri Nesterov (1998), Springer Publishing, **Introductory Lectures on Convex Optimization: A Basic Course**

Convergence lower bounds strongly convex

Theorem (Nesterov)

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$$\min_{i=1,\ldots,T} f(w^i) - f(w^*) \geq \frac{3L\|w^1 - w^*\|_2^2}{32(T+1)^2} = O\left(\frac{1}{T^2}\right).$$

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Exercises !

Solve ridge_reg_exe.pdf

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