Gradient descent : theory and practice

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Slides courtesy of Robert Gower

Machine learning task

Finite Sum Training Problem

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

Today: assume that f is differentiable and L-smooth

! ∇f exists

Iterative minimization

Finite Sum Training Problem

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

Usually cannot solve this in closed form : $\quad w^* = \ldots$

Idea: start from initial guess w^0 and try to find a new, better point. Iterative process $\quad w^0 \rightarrow w^1 \rightarrow \ldots$

Gradient descent : basic idea

Given w^0, look for w^1 as $w^1 = w^0 + d$ where d is a small displacement.

Ideally: $$d \in \arg\min_{d \in \mathbb{R}^p} f(w^0 + d)$$

Just as hard as the original problem :(

Solution: $$d \in \arg\min_{\|d\| \leq \varepsilon} f(w^0 + d)$$

Q: as ε goes to 0, what is the limit of d ?

Gradient descent algorithm

Init : Select initial guess w^0

For t = 0, 1, ..., T:

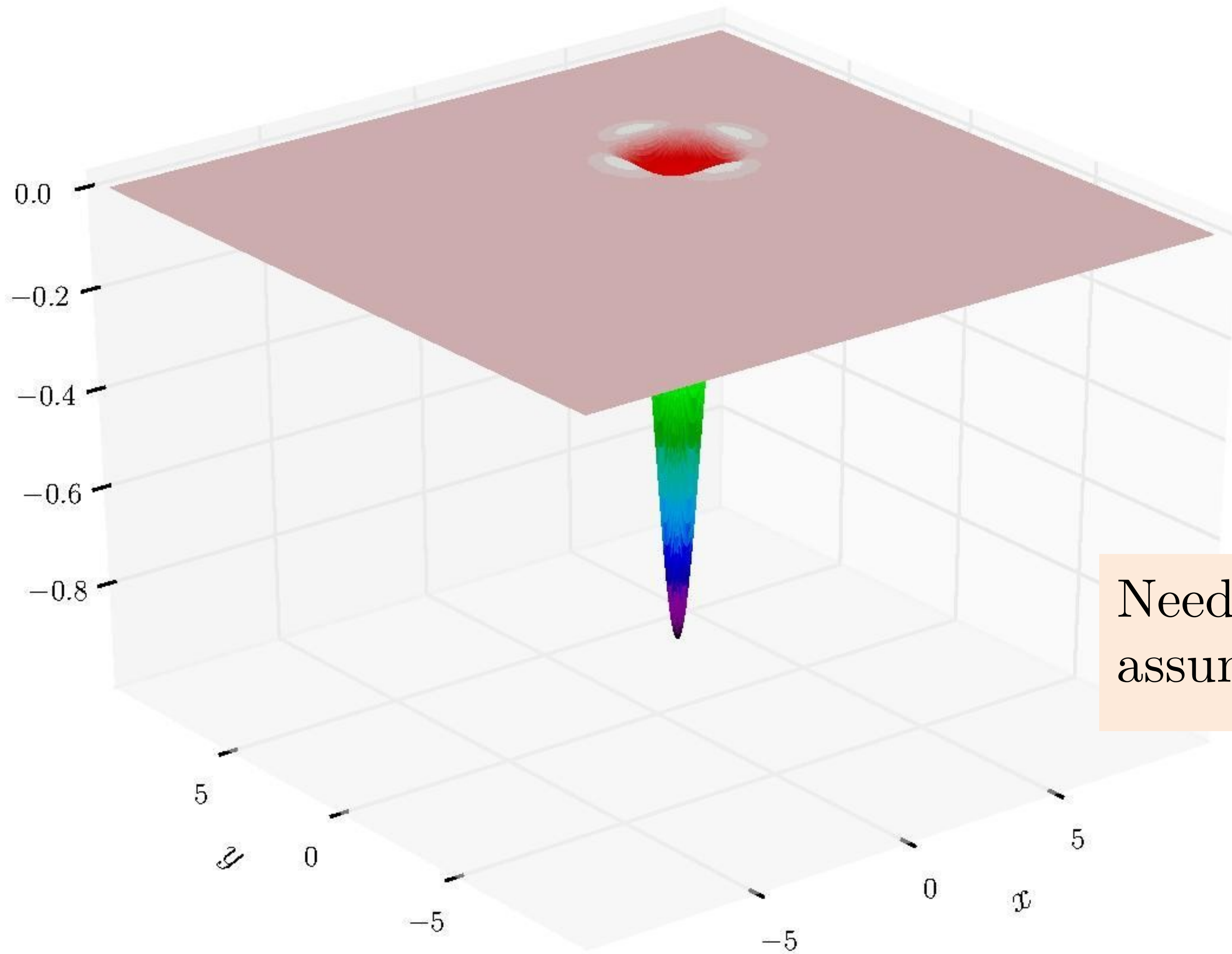
- Select a step size $\rho^t \in \mathbb{R}^+$
- Update $w^{t+1} = w^t - \rho^t \nabla f(w^t)$

Return : w^{T+1}

Questions :

- Does it converge? In which sense?
- At which speed?
- Choice of ρ^t?

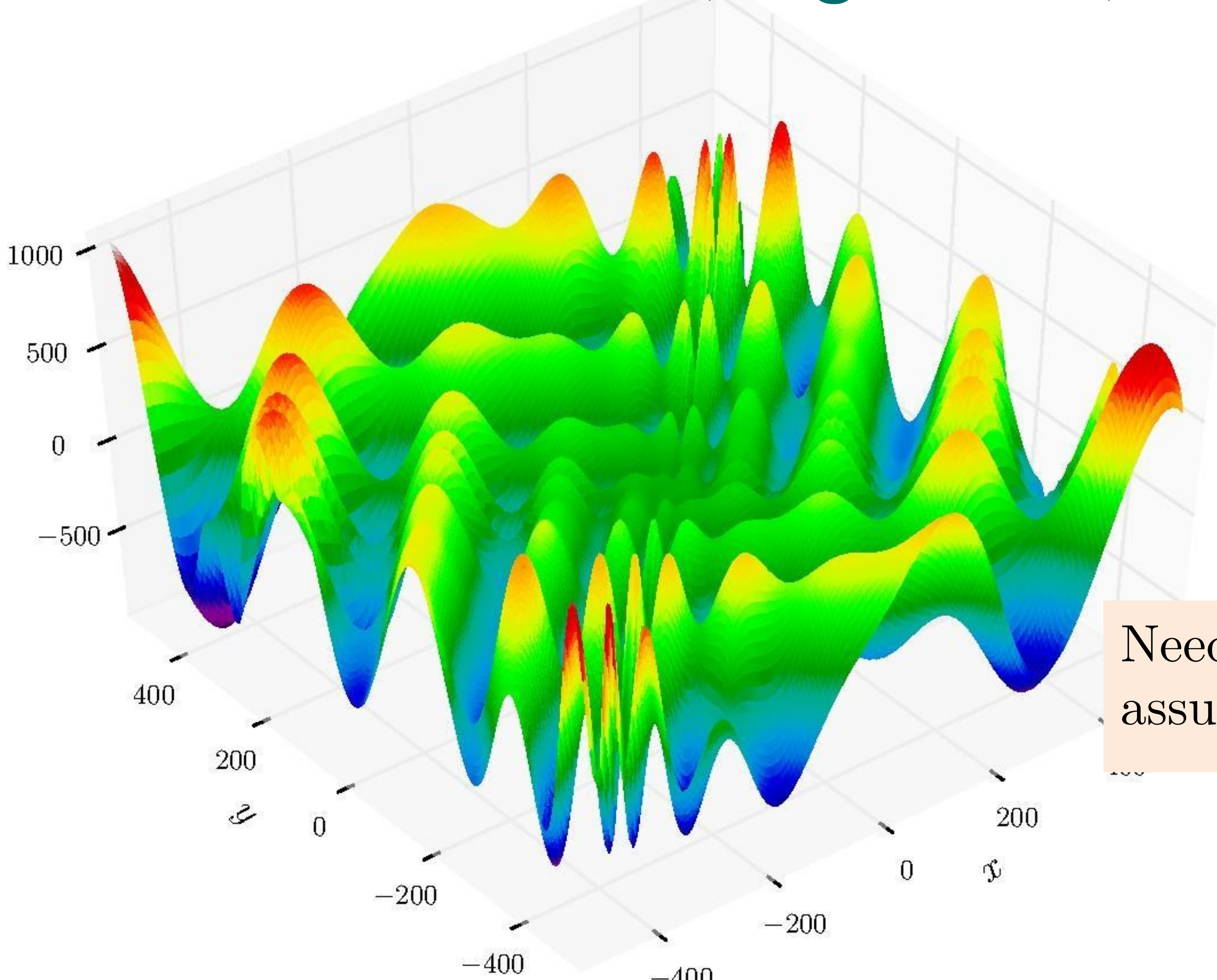
Optimization is hard (in general)



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!

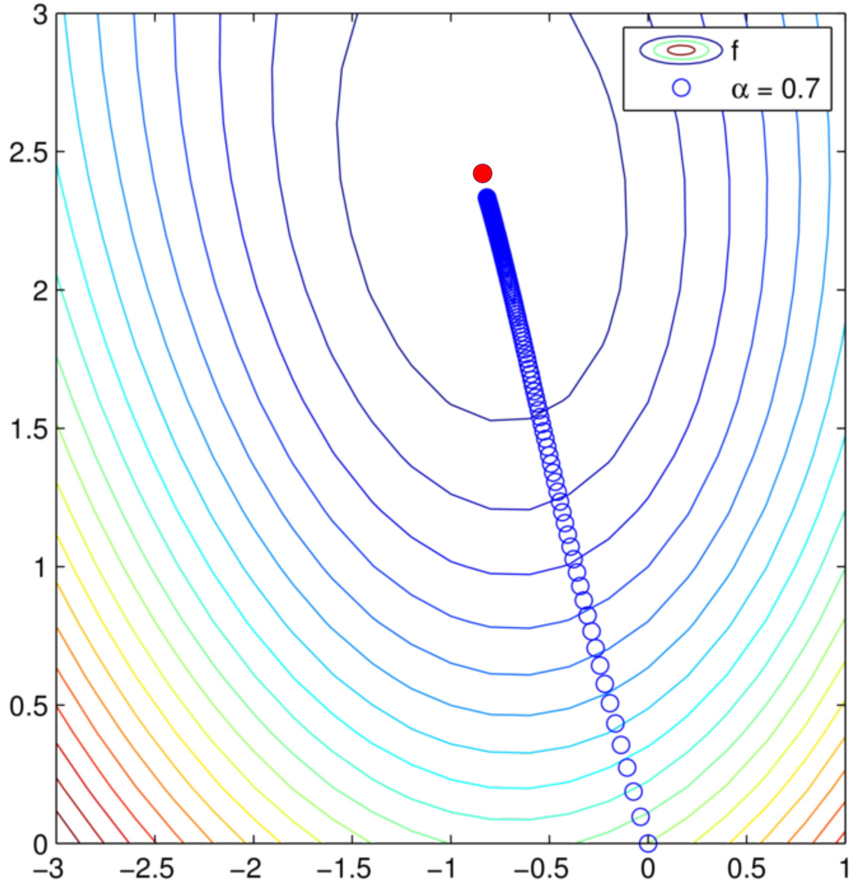
$$f(x, y) = -(y + 47)\sin\sqrt{\left|\tfrac{x}{2} + (y + 47)\right|} - x\sin\sqrt{\left|\tfrac{x}{2} - (y + 47)\right|}$$

Gradient Descent Example

A Logistic Regression problem using the fourclass labelled data from LIBSVM
$(n,\ d) = (862{,}2)$

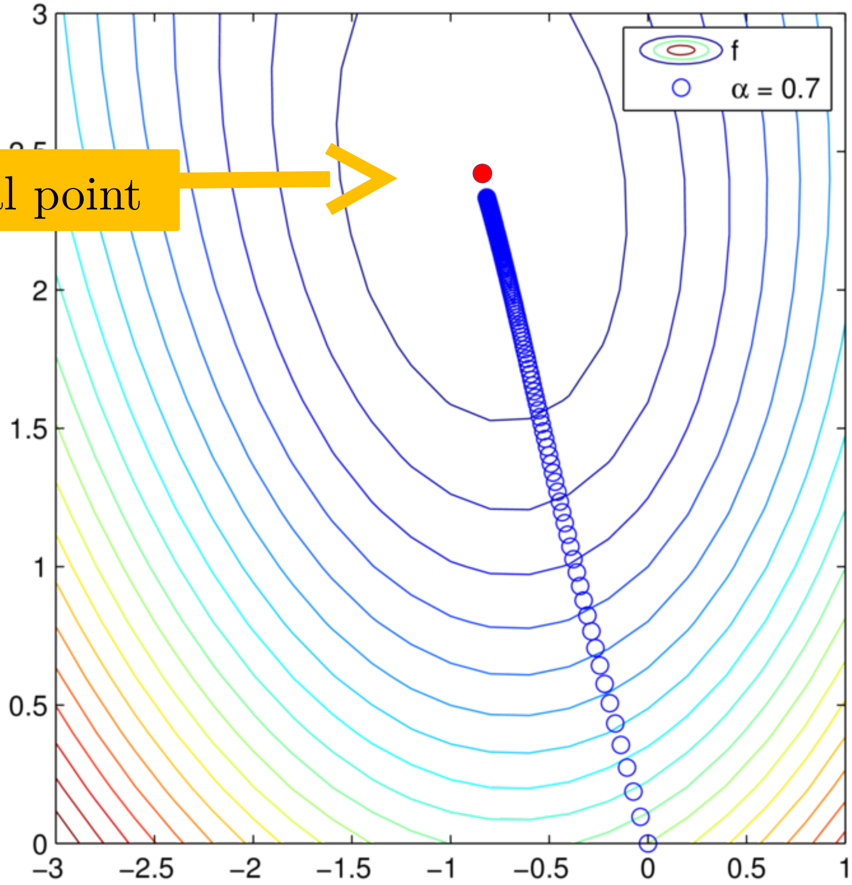
Logistic Regression

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



Can we prove that this always works?

Gradient Descent Example



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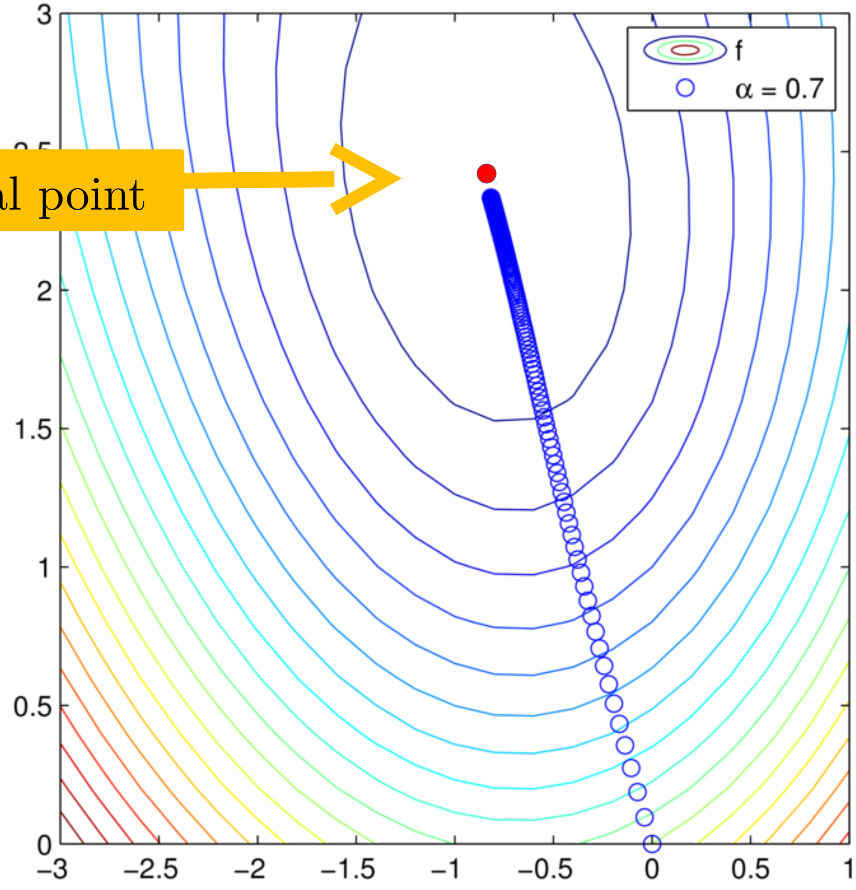
Gradient Descent Example

Optimal point



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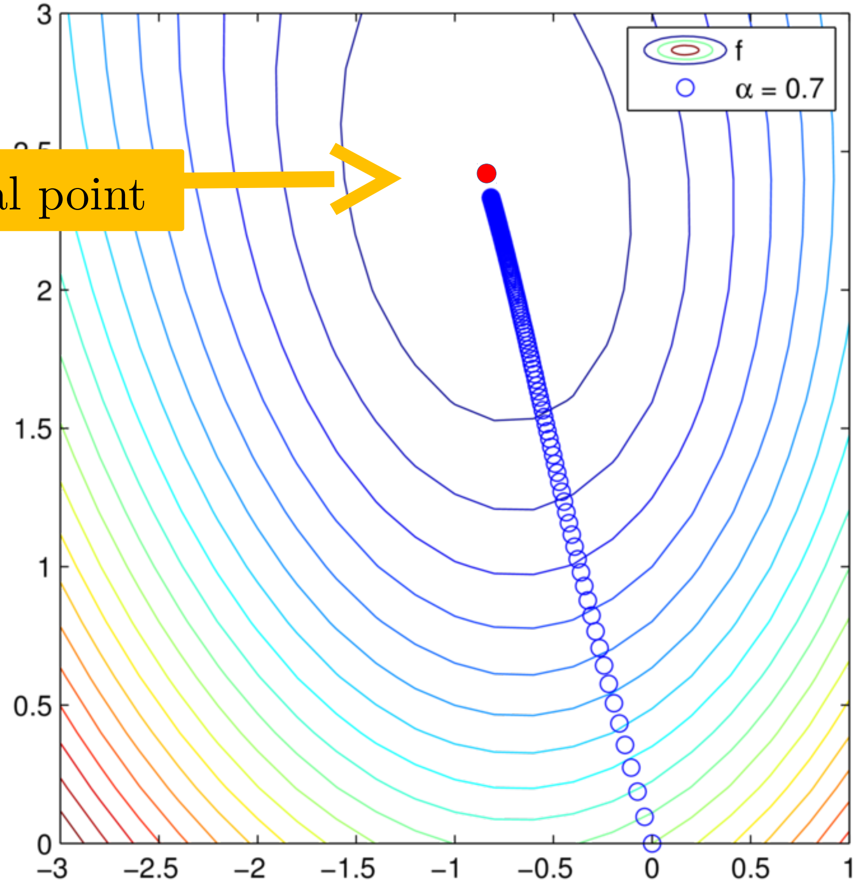
Can we prove that this always works?

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

Gradient Descent Example



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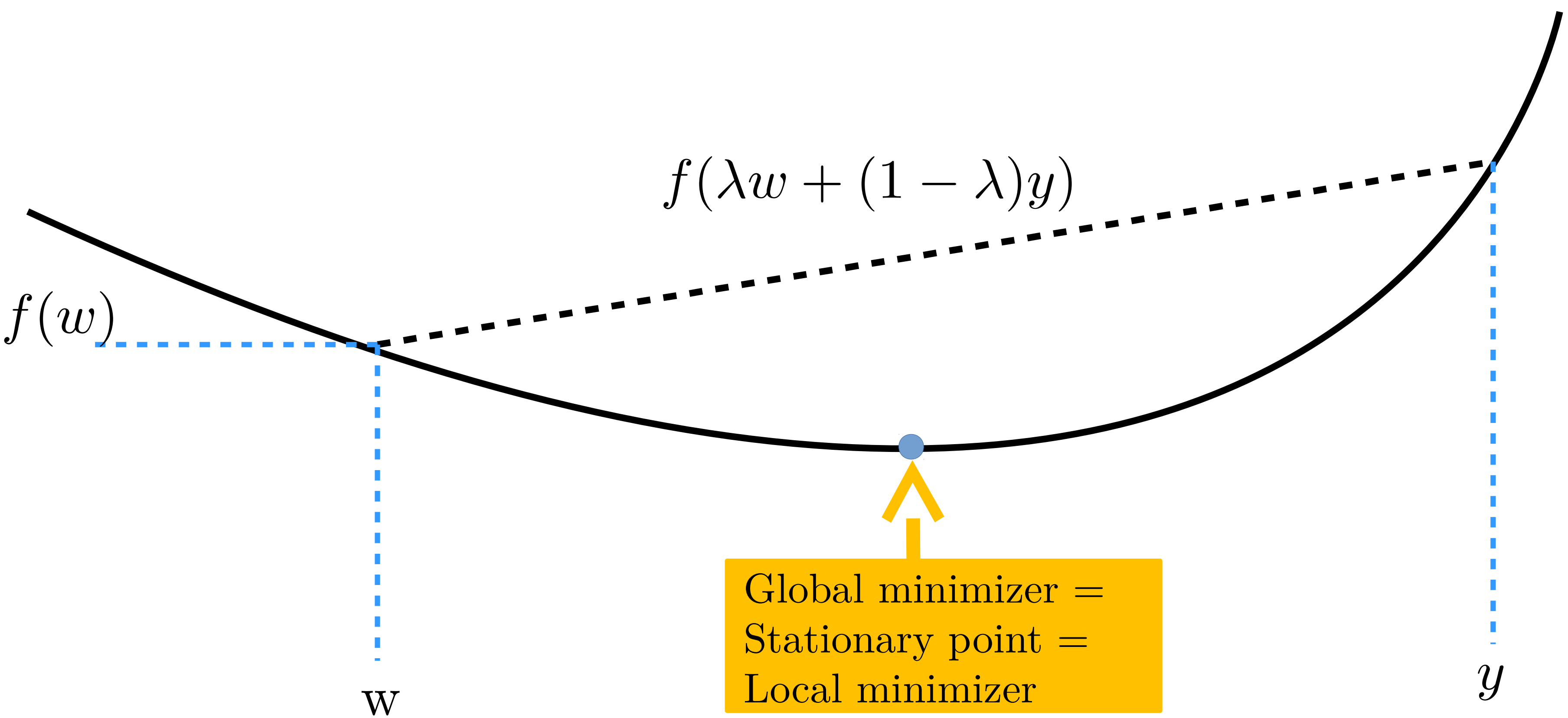
Specialize

Convex and smooth training problems

Convexity

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

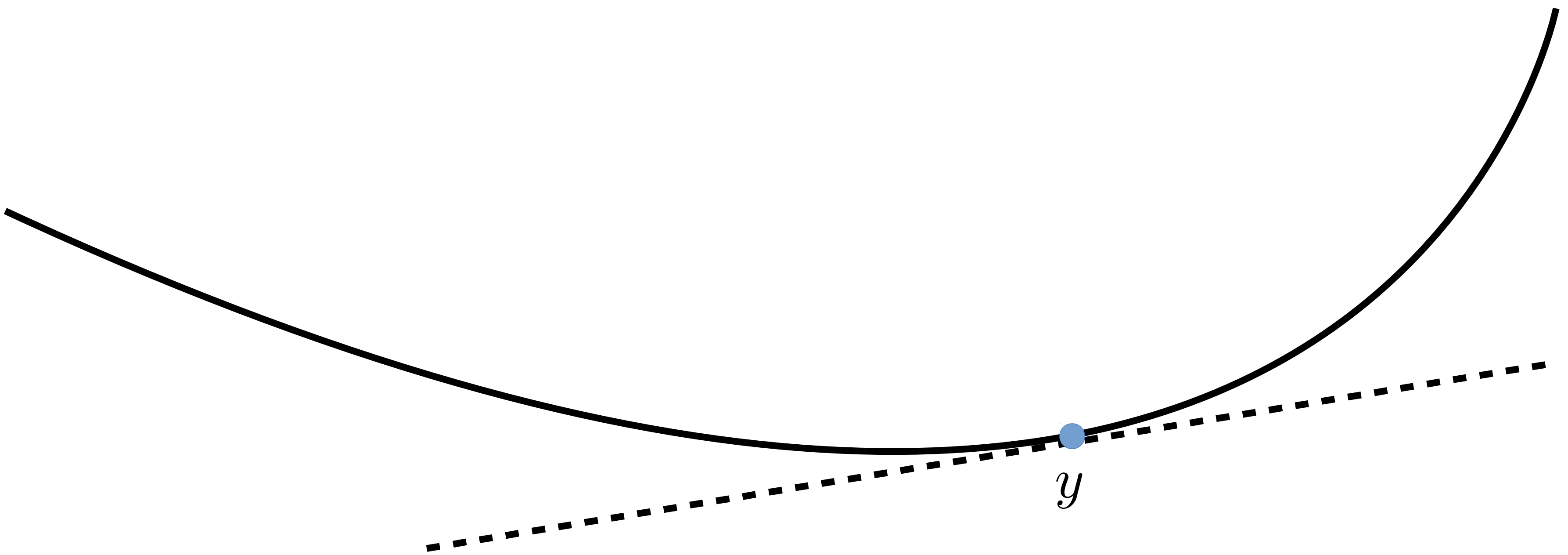
$$f(\lambda w + (1-\lambda)y) \leq \lambda f(w) + (1-\lambda)f(y), \quad \forall w, y \in C, \lambda \in [0,\, 1]$$



Convexity

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

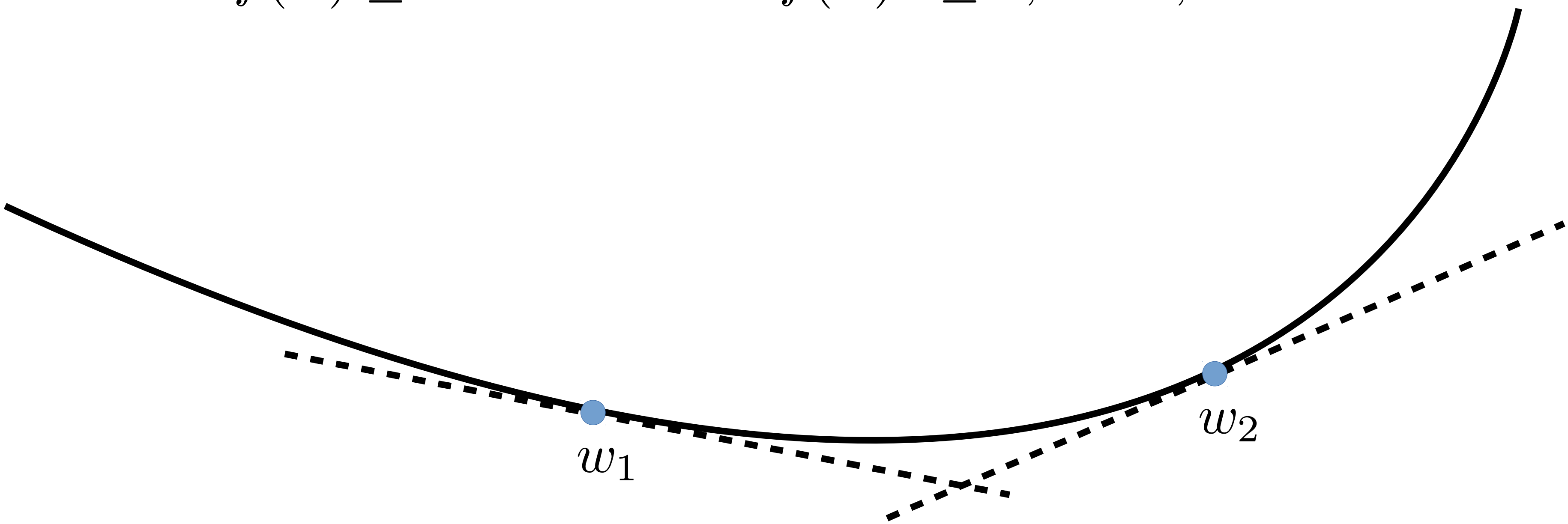
$$f(w) \geq f(y) + \langle \nabla f(y), w - y \rangle$$



Convexity

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

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



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

Main Advantage of Convexity

Nice Property

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

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All stationary points are global minima

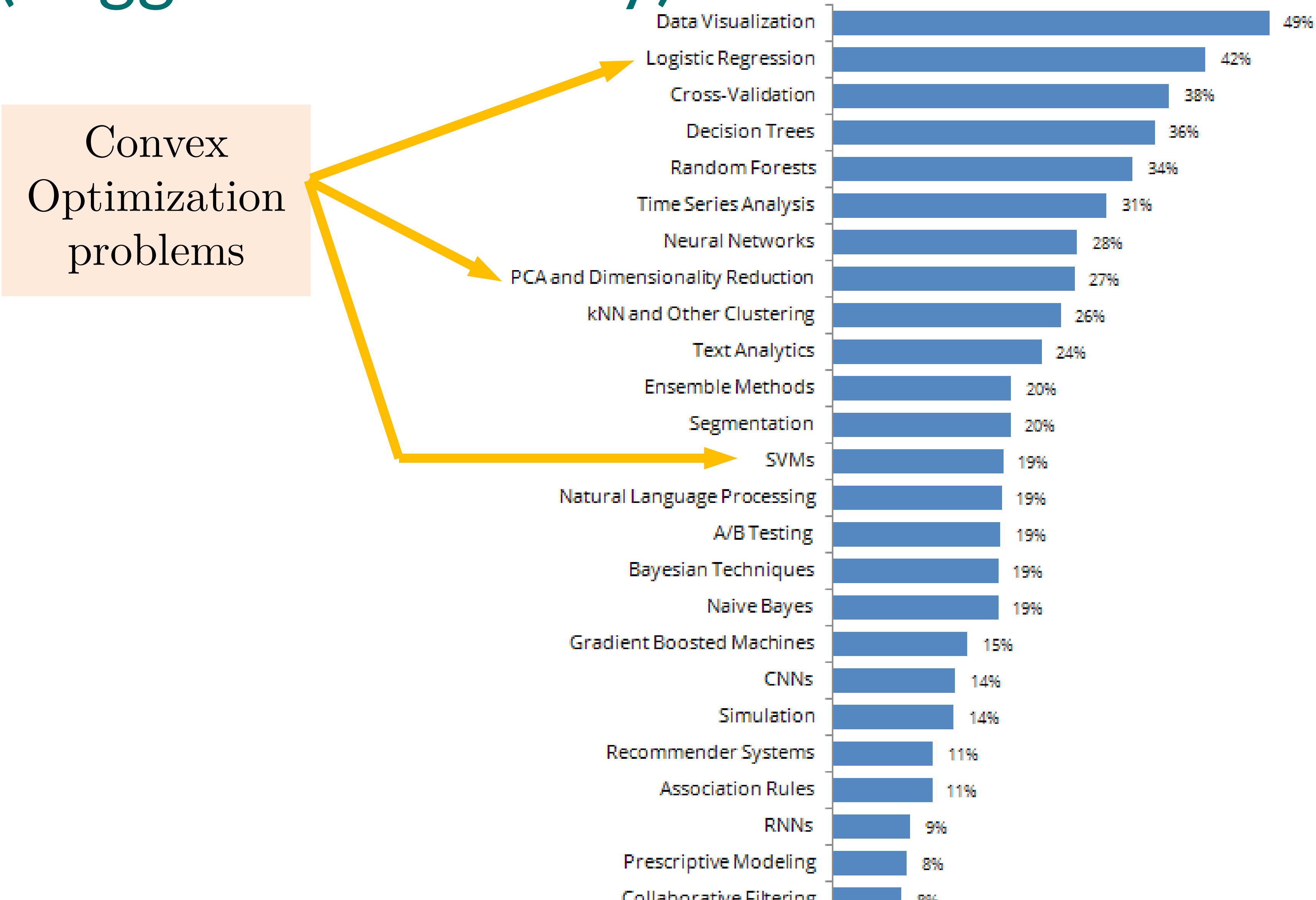
Lemma: Convexity => Nice property

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

then Nice Property holds

PROOF: Choose $y = w^*$

Data science methods most used (Kaggle 2017 survey)



Convexity: Examples

Extended-value extension:

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

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

Norms and squared norms:

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

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

Negative log and logistic:

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

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

Hinge loss

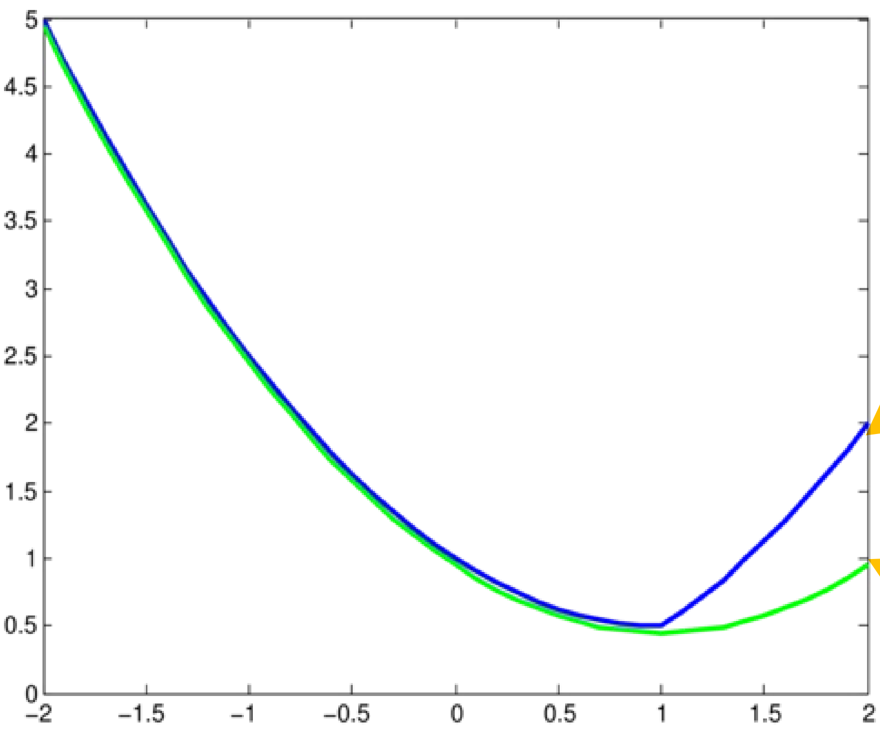
$$x \mapsto \max\{0, 1 - yx\}$$

Negatives log determinant, exponentiation ... etc

Strong convexity

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

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



Hinge loss + L2

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

Quadratic lower bound

Smoothness

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

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

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

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

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

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

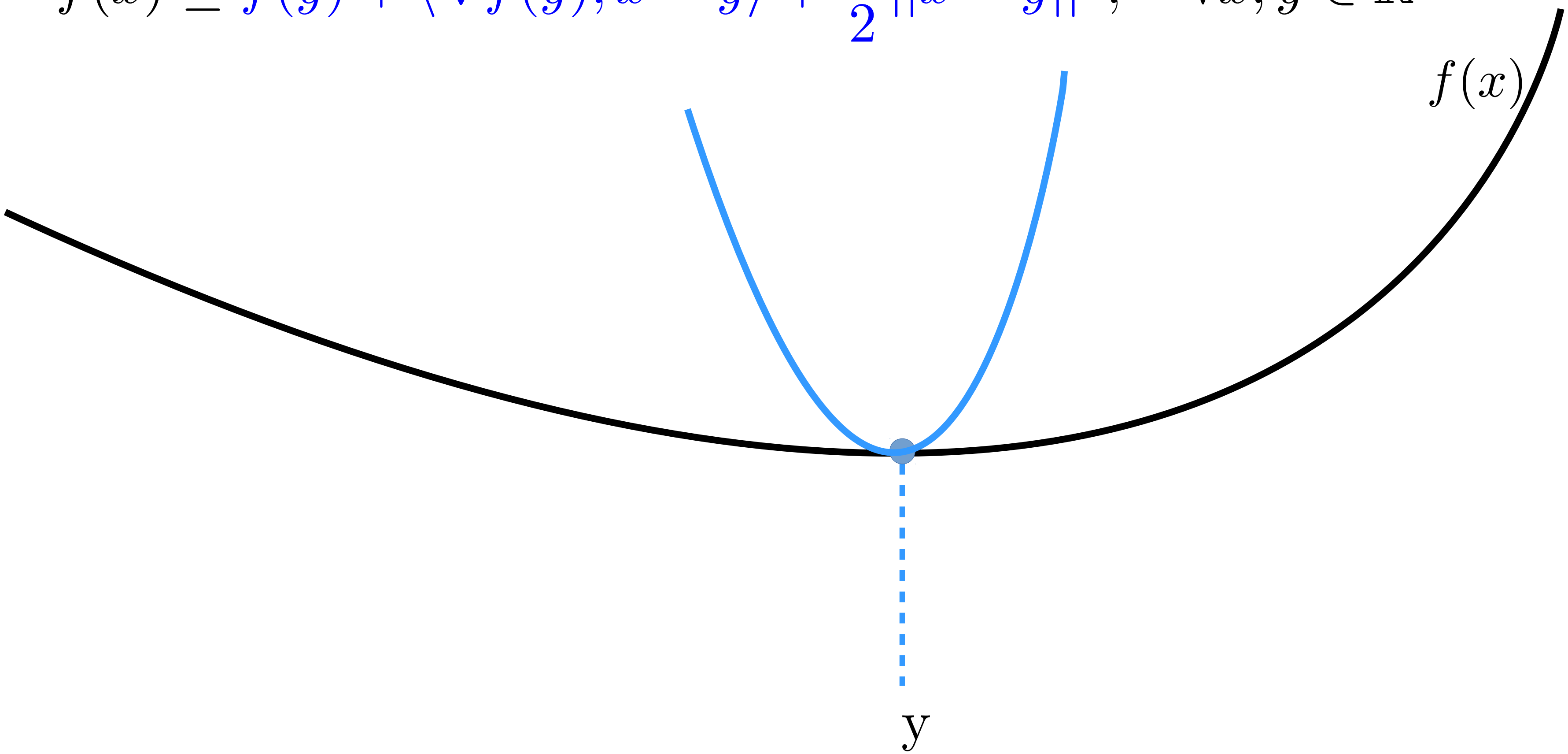
EXE: determine the strong convexity / smoothness constants of

$$f(w) := \tfrac{1}{2}||X^\top w - b||_2^2 \text{ for } X \in \mathbb{R}^{n \times p}, \; b \in \mathbb{R}^n$$

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: Examples

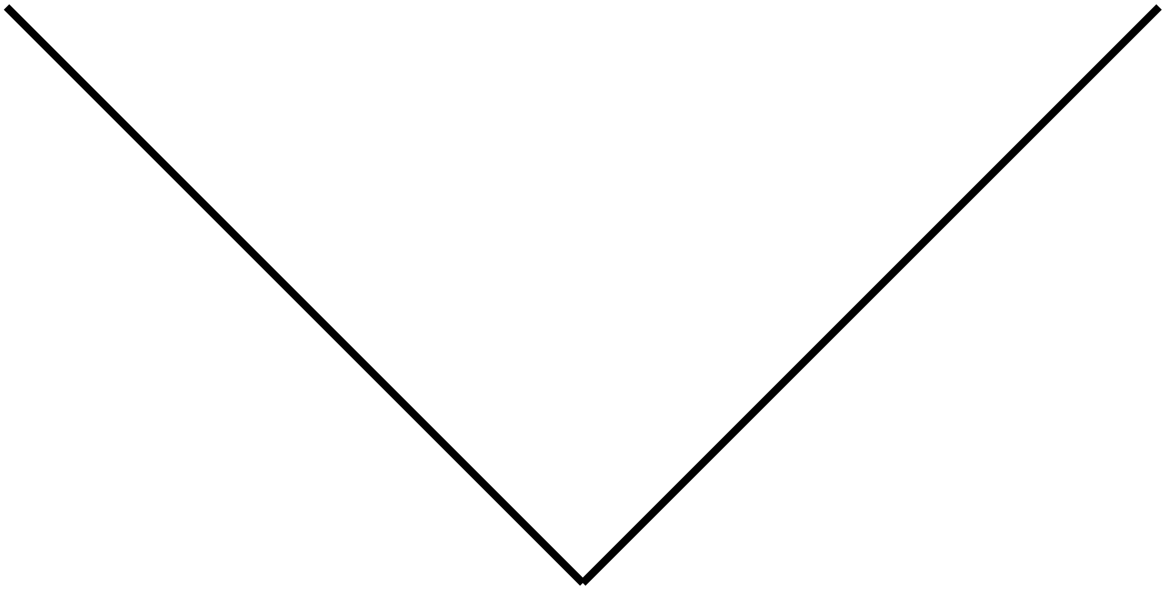
Convex quadratics: $x \mapsto x^\top A x + b^\top x + c$

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

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

Smoothness: Convex counter-example

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



We'll see how to handle this problem next class

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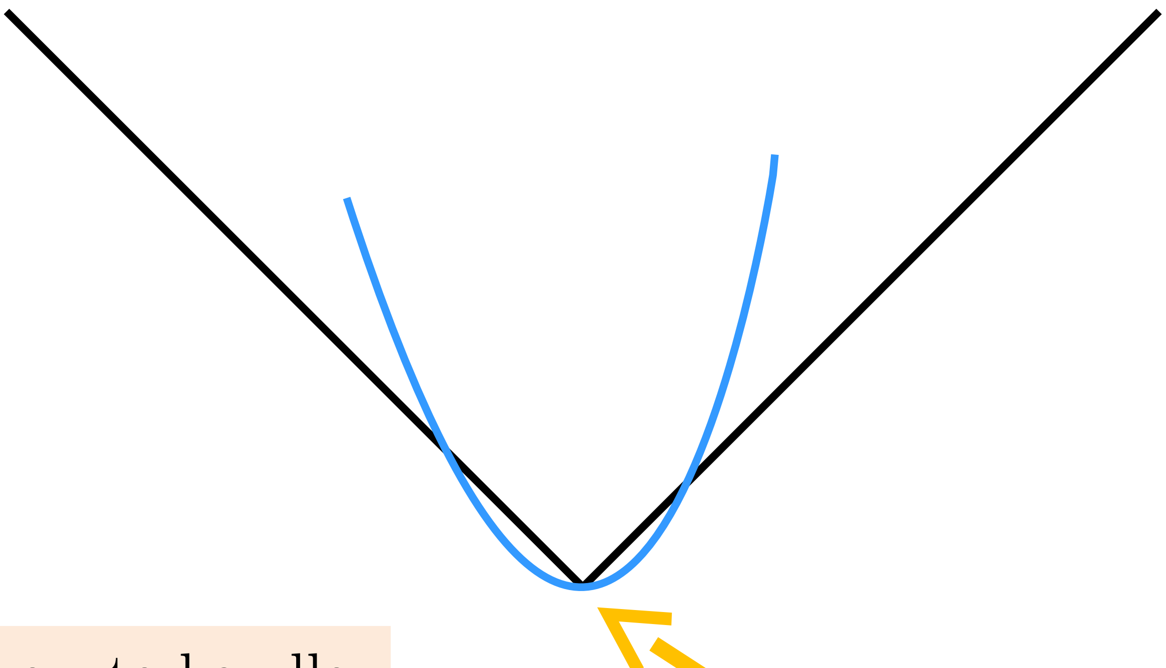

We'll see how to handle this problem next class

Does not fit
Not smooth

Insight into Gradient Descent using Smoothness

$$f(w) \leq f(w^0) + \langle \nabla f(w^0), w - w^0 \rangle + \frac{L}{2} ||w - w^0||^2$$

Q: what is the minimizer of the upper bound in w?

Insight into Gradient Descent using Smoothness

$$\boxed{f(w) \leq f(w^0) + \langle \nabla f(w^0), w - w^0 \rangle + \frac{L}{2} ||w - w^0||^2}$$

Minimizing the upper bound in w we get:

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

A gradient descent step !

$$w = w^0 - \frac{1}{L} \nabla f(w^0)$$

Insight into Gradient Descent using Smoothness

$$\boxed{f(w) \leq f(w^0) + \langle \nabla f(w^0), w - w^0 \rangle + \frac{L}{2}||w - w^0||^2}$$

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

$$w = w^0 - \frac{1}{L}\nabla f(w^0)$$

A gradient descent step !

Convergence rates: smooth case

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

Gradient descent with step $\rho^t = \frac{1}{L}$:

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

$$\sum_{t=0}^{T} \|\nabla f(w^t)\|^2 \leq 2L(f(w^0) - f(w^*)), \ \ \forall T > 0$$

Q: what does it mean?

Convergence rates: smooth case

Theorem : if f is L-smooth, the iterates of gradient descent verify

$$\nabla f(w^t) \to 0$$

$$\inf_{t \leq T} \|\nabla f(w^t)\|^2 \leq \frac{2L}{T}(f(w^0) - f(w^*))$$

Convergence speed

Slow convergence

Say $2L(f(w^0) - f(w^*)) = 1$

In order to have $\inf_{t \leq T} \|\nabla f(w^t)\|^2 \leq 10^{-4}$

Need 10^4 iterations...

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

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

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

Convergence GD strongly convex

Theorem

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

$$f(w^t) - f(w^*) \leq (1 - \frac{\mu}{L})^t (f(w^0) - f(w^*))$$

Where

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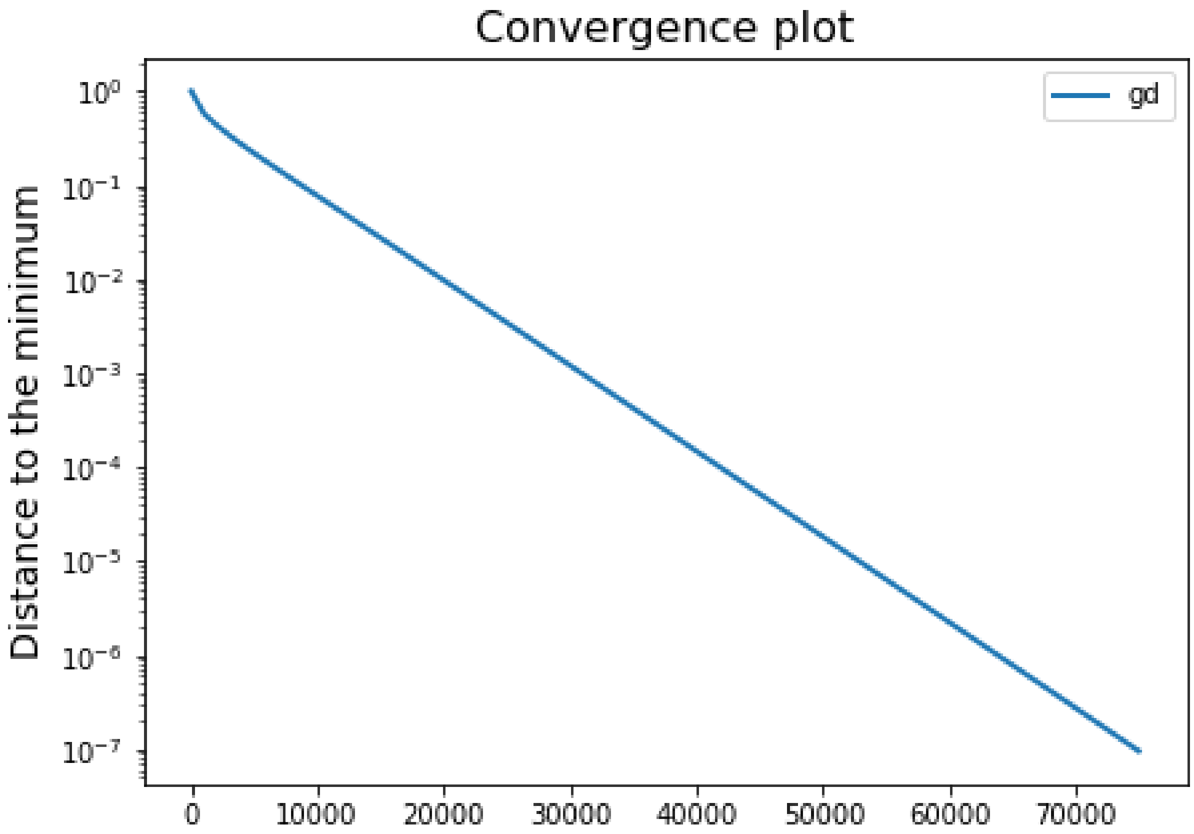
Gradient Descent Example: logistic regression



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

Proof Convergence GD strongly convex + smooth

Smoothness

Proof:

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

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

Proof Convergence GD strongly convex + smooth

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

Polyak-Lojasiewicz (PL) inequality :

Q: show that strong convexity => PL

$$\|\nabla f(w)\|^2 \geq 2\mu(f(w) - f(w^*)), \quad \forall w$$

Proof Convergence GD strongly convex + smooth

Smoothness

Proof:

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

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

Polyak-Lojasiewicz (PL) inequality :

$$\|\nabla f(w)\|^2 \geq 2\mu(f(w) - f(w^*)), \quad \forall w$$

$$f(w^{t+1}) \leq f(w^t) - \frac{\mu}{L}(f(w^t) - f(w^*))$$

$$f(w^t) - f(w^*) \leq (1 - \frac{\mu}{L})^t (f(w^0) - f(w^*))$$

Examples of smooth machine learning problems

Least squares

Data: $x_1, \ldots x_n \in \mathbb{R}^p$, and $y_1, \ldots, y_n \in \mathbb{R}$

Assumption: There exists w^* such that

$$y_i \simeq \langle x_i, w^* \rangle$$

Optimization problem: $\min_w f(w) = \frac{1}{n} \sum_{i=1}^{n} (\langle x_i, w \rangle - y_i)^2$

Q: show that we can rewrite $f(w) = \frac{1}{n} \|Xw - y\|^2$

Is the problem convex, smooth? Compute the associated constants

Ridge regression

Problem :

$$\min_w f(w) = \frac{1}{n}\sum_{i=1}^{n}(\langle x_i, w\rangle - y_i)^2$$

Has infinitely many solutions when n < p. Bad conditioning, and very sensitive to X.

Solution : regularize !

$$\min_w f(w) = \frac{1}{n}\sum_{i=1}^{n}(\langle x_i, w\rangle - y_i)^2 + \frac{\lambda}{2}\|w\|^2$$

Q: Is the problem convex, smooth? Compute the associated constants

Logistic regression

Data: $x_1, \ldots x_n \in \mathbb{R}^p$, and $y_1, \ldots, y_n \in \{-1, +1\}$

Assumption: There exists w^* such that

$$y_i \simeq \mathrm{sign}(\langle x_i, w^* \rangle)$$

Optimization problem:

$$\min_w f(w) = \frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-y_i \langle x_i, w \rangle))$$

Q: Is the problem convex, smooth? Compute the associated constants

Regularized logistic regression

Data: $x_1, \dots x_n \in \mathbb{R}^p$, and $y_1, \dots, y_n \in \{-1, +1\}$

Assumption: There exists w^* such that

$$y_i \simeq \operatorname{sign}(\langle x_i, w^* \rangle)$$

Optimization problem:

$$\min_w f(w) = \frac{1}{n} \sum_{i=1}^n \log(1 + \exp(-y_i \langle x_i, w \rangle)) + \frac{\lambda}{2} \|w\|^2$$

Q: Is the problem convex, smooth? Compute the associated constants