Optimization

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Journées YSP

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Outline

1. **General context and examples.**
2. **What makes optimization hard ?**

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2. What makes optimization hard ?

   In the context of supervised machine learning:

3. Minimizing Empirical Risk.

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2. What makes optimization hard ?

In the context of supervised machine learning:

3. Minimizing Empirical Risk.
4. Minimizing Generalization Risk.

General context

What is optimization about ?

$$\min_{\theta \in \Theta} f(\theta)$$

With θ a parameter, and f a cost function.

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With θ a parameter, and f a cost function.

Why ?
We formulate our problem as an optimization problem.
3 examples:

- Supervised machine learning
- Signal Processing
- Optimal transport

Some Examples

Example 1: Supervised Machine Learning

Goal: predict a phenomenon from "explanatory variables", given a set of observations.

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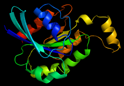

Bio-informatics

Input: DNA/RNA sequence,
Output: Drug responsiveness

Image classification

Input: Images,
Output: Digit

Supervised Machine Learning

Example 1: Supervised Machine Learning

Consider an input/output pair $(X, Y) \in \mathcal{X} \times \mathcal{Y}$, $(X, Y) \sim \rho$.

Goal: function $\theta : \mathcal{X} \to \mathbb{R}$, s.t. $\theta(X)$ good prediction for Y.

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Consider a loss function $\ell : \mathcal{Y} \times \mathbb{R} \to \mathbb{R}_+$

Define the Generalization risk :

$$\mathcal{R}(\theta) := \mathbb{E}_\rho \left[\ell(Y, \langle \theta, \Phi(X) \rangle) \right].$$

Empirical Risk minimization (I)

Data: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \ldots, n$, i.i.d.

Empirical risk (or training error):

$$\hat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \langle \theta, \Phi(x_i) \rangle).$$

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Empirical risk minimization (ERM) : find $\hat{\theta}$ solution of

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} \ell\big(y_i, \langle \theta, \Phi(x_i) \rangle\big) \quad + \quad \mu \Omega(\theta).$$

convex data fitting term + regularizer

Empirical Risk minimization (II)

For example, least-squares regression:

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{2n} \sum_{i=1}^{n} \big(y_i - \langle \theta, \Phi(x_i) \rangle\big)^2 \quad + \quad \mu \Omega(\theta),$$

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and logistic regression:

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} \log \big(1 + \exp(-y_i \langle \theta, \Phi(x_i) \rangle)\big) \quad + \quad \mu \Omega(\theta).$$

Some Examples

Example 2: Signal processing

Observe a signal $Y \in \mathbb{R}^{n \times q}$, try to recover the source $B \in \mathbb{R}^{p \times q}$, knowing the "forward matrix" $X \in \mathbb{R}^{n \times p}$. (multi-task regression)

$$\min_{\beta} \|X\beta - Y\|_F^2$$

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Ω sparsity inducing regularization.

How to choose λ?

Some Examples

Example 3: Optimal transport

$$\min_{\pi \in \Pi} \int c(x,y) \mathrm{d}\pi(x,y)$$

Π set of probability distributions $c(x,y)$ “distance” from x to y.

$+$ regularization

Kantorovic formulation of OT.

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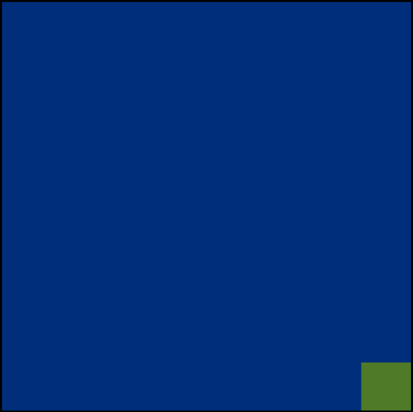

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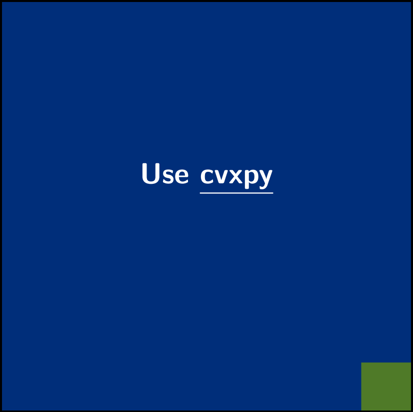

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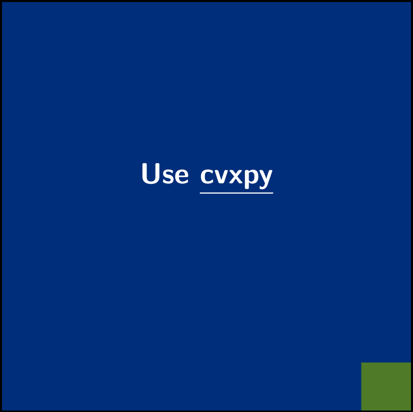

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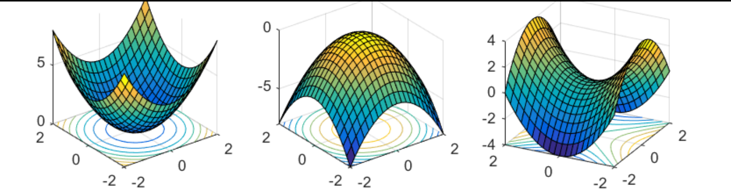
Interesting (or hard) problems

What makes it hard: 1. Convexity

Why?



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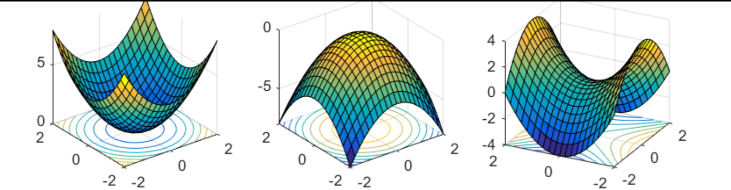

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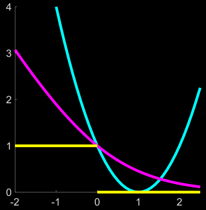
Empirical risk minimization with 0-1 loss.



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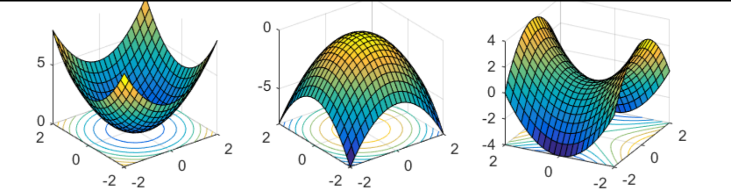

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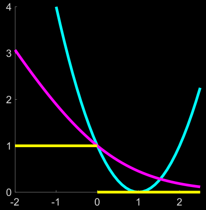

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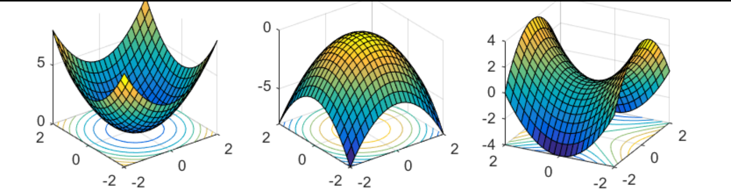

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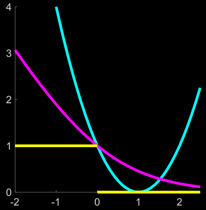

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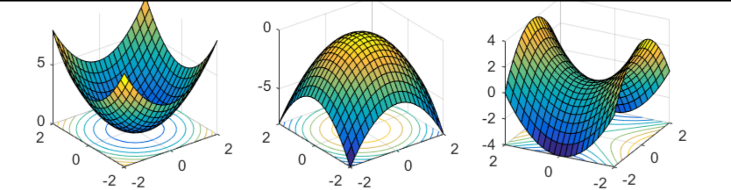

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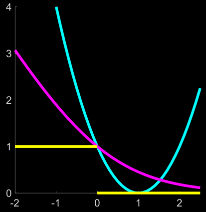

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Neural networks: parametric non-convex functions.

What makes it hard: 2. Regularity of the function

a. Smoothness

- A function $g : \mathbb{R}^d \to \mathbb{R}$ is L-smooth if and only if it is twice differentiable and

$$\forall \theta \in \mathbb{R}^d, \text{ eigenvalues}\big[g''(\theta)\big] \leqslant L$$

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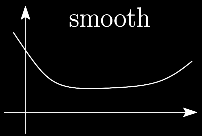

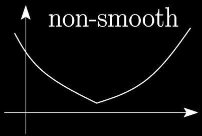

For all $\theta \in \mathbb{R}^d$:

$$g(\theta) \leq g(\theta') + \langle g(\theta'), \theta - \theta' \rangle + L \left\| \theta - \theta' \right\|^2$$

What makes it hard: 2. Regularity of the function

b. Strong Convexity

- A twice differentiable function $g : \mathbb{R}^d \to \mathbb{R}$ is μ-strongly convex if and only if

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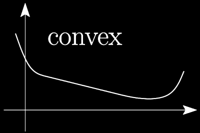

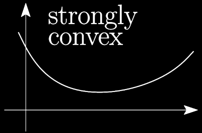

For all $\theta \in \mathbb{R}^d$:

$$g(\theta) \geq g(\theta') + \langle g(\theta'), \theta - \theta' \rangle + \mu \left\|\theta - \theta'\right\|^2$$

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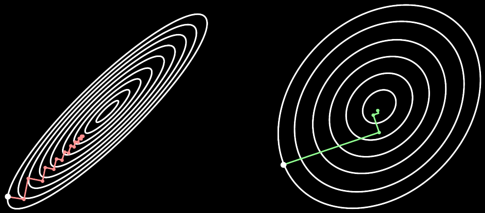
Rates typically depend on the condition number $\kappa = \frac{L}{\mu}$:



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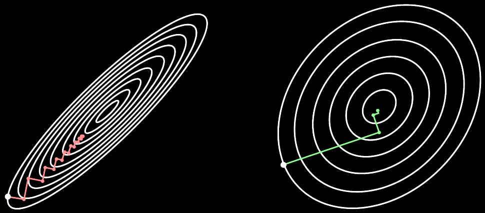

Large κ
harder to optimize

Small κ
easier to optimize

Smoothness and strong convexity in ML

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Note: when considering dual formulation of the problem:

- L-smoothness $\leftrightarrow$ $1/L$-strong convexity.
- μ-strong convexity $\leftrightarrow$ $1/\mu$-smoothness

What makes it hard: 3. Set Θ, complexity of f

a. **Set Θ:** (if Θ is a convex set.)

- May be described implicitly (via equations):
  $\Theta = \{\theta \in \mathbb{R}^d$ s.t. $\|\theta\|_2 \leq R$ and $\langle \theta, 1 \rangle = r\}$.

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b. Structure of f. If $f = \hat{\mathcal{R}}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, \langle \theta, \Phi(x_i) \rangle)$, computing a gradient has a cost proportional to n.

Optimization

Take home

- We express problems as minimizing a function over a set
- Most convex problems are solved
- Difficulties come from non-convexity, lack of regularity, complexity of the set Θ (or high dimension), complexity of computing gradients

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What happens for supervised machine learning ? Goals:

- present algorithms (convex, large dimension, high number of observations)
- show how rates depend onsmoothness and strong convexity
- show how we can use the structure
- not forgetting the initial problem...!

Stochastic algorithms for ERM

$$\min_{\theta \in \mathbb{R}^d} \left\{ \hat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \langle \theta, \Phi(x_i) \rangle) \right\}.$$

Two fundamental questions: (a) computing (b) analyzing $\hat{\theta}$.

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"Large scale" framework: number of examples n and the number of explanatory variables d are both large.

1. High dimension d $\Longrightarrow$ First order algorithms

Gradient Descent (GD) :

$$\boxed{\theta_k = \theta_{k-1} - \gamma_k \hat{\mathcal{R}}'(\theta_{k-1})}$$

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Problem: computing the gradient costs $O(dn)$ per iteration.

2. Large $n \implies$ Stochastic algorithms

Stochastic Gradient Descent (SGD)

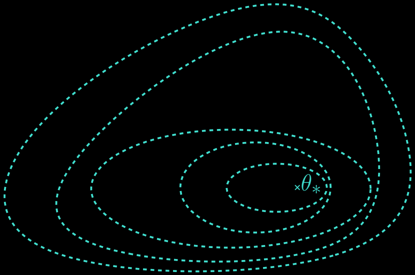
Stochastic Gradient descent

- **Goal:**

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

  given unbiased gradient estimates f'_n

- $\theta_* := \mathrm{argmin}_{\mathbb{R}^d} f(\theta)$.



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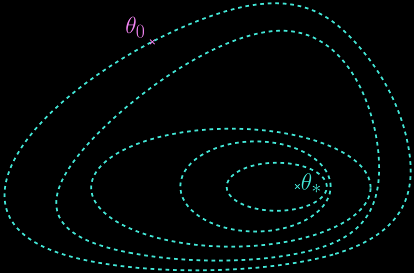

- $\theta_* := \mathrm{argmin}_{\mathbb{R}^d} f(\theta)$.
- Key algorithm: Stochastic Gradient Descent (SGD) (Robbins and Monro, 1951):

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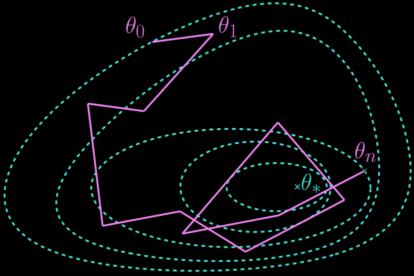
Stochastic Gradient descent

- **Goal:**

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

  given unbiased gradient estimates f'_n
- $\theta_* := \mathrm{argmin}_{\mathbb{R}^d} f(\theta)$.



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SGD for ERM: $f = \hat{\mathcal{R}}$

Loss for a single pair of observations, for any $j \le n$:

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with $\mathcal{F}_k = \sigma((x_i, y_i)_{1 \leq i \leq n}, (I_i)_{1 \leq i \leq k})$.

Analysis: behaviour of $(\theta_n)_{n\geq 0}$

$$\boxed{\theta_k = \theta_{k-1} - \gamma_k f_k'(\theta_{k-1})}$$

Importance of the learning rate $(\gamma_k)_{k\geq 0}$.

For smooth and strongly convex problem, $\theta_k \to \theta_*$ a.s. if

$$\sum_{k=1}^{\infty} \gamma_k = \infty \qquad \sum_{k=1}^{\infty} \gamma_k^2 < \infty.$$

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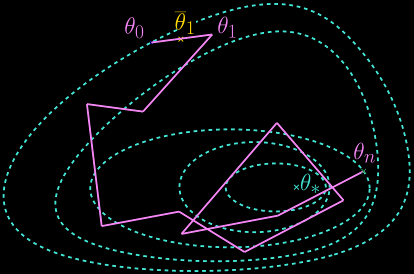
- Limit variance scales as $1/\mu^2$
- Very sensitive to ill-conditioned problems.
- μ generally unknown...

Polyak Ruppert averaging



Introduced by Polyak and Juditsky (1992) and Ruppert (1988):

$$\bar{\theta}_k = \frac{1}{k+1}\sum_{i=0}^{k}\theta_i.$$

- **off line averaging reduces the noise effect.**

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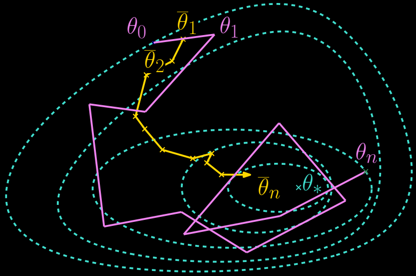

- off line averaging reduces the noise effect.
- on line computing: $\bar{\theta}_{k+1} = \frac{1}{k+1}\theta_{k+1} + \frac{k}{k+1}\bar{\theta}_k$.

Convex stochastic approximation: convergence

Known global minimax rates for non-smooth problems

- Strongly convex: $O((\mu k)^{-1})$
  Attained by averaged stochastic gradient descent with $\gamma_k \propto (\mu k)^{-1}$
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For smooth problems

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  for $\gamma_k \propto k^{-1/2}$: adapts to strong convexity.

Convergence rate for $f(\tilde{\theta}_k) - f(\theta_*)$, smooth f.

	$\min \hat{\mathcal{R}}$	
	SGD	GD
Convex	$O\left(\frac{1}{\sqrt{k}}\right)$	$O\left(\frac{1}{k}\right)$

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Can we get best of both worlds ?

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↬ ⊕ update costs the same as SGD

↬ ⊖ needs to store all gradients $f_i'(\theta_{k_i})$ at "points in the past"

Some references:

- SAG Schmidt et al. (2013), SAGA Defazio et al. (2014a)
- SVRG Johnson and Zhang (2013) (reduces memory cost but 2 epochs...)
- FINITO Defazio et al. (2014b)
- S2GD Konečný and Richtárik (2013)...

And many others... See for example Niao He's lecture notes for a nice overview.

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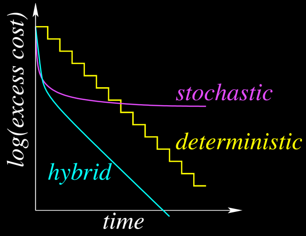

GD, SGD, SAG (Fig. from Schmidt et al. (2013))

Take home

Stochastic algorithms for Empirical Risk Minimization.

- **Rates depend on the regularity of the function.**
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- **Stochastic algorithms** to optimize a **deterministic function**.

What about generalization risk

Initial problem: Generalization guarantees.

- Uniform upper bound $\sup_\theta \left| \hat{\mathcal{R}}(\theta) - \mathcal{R}(\theta) \right|$. (empirical process theory)
- More precise: localized complexities (Bartlett et al., 2002), stability (Bousquet and Elisseeff, 2002).

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	ERM minimization	Gen. risk minimization
	several passes : $0 \leq k$	One pass $0 \leq k \leq n$
x_i, y_i is	$\mathcal{F}_t$-measurable for any t	$\mathcal{F}_t$-measurable for $t \geq i$.

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Gradient is unknown

Least Mean Squares: rate independent of μ

Least-squares: $\mathcal{R}(\theta) = \frac{1}{2}\mathbb{E}\big[(Y - \langle \Phi(X), \theta\rangle)^2\big]$

Analysis for averaging and constant step-size $\gamma = 1/(4R^2)$ (Bach and Moulines, 2013)

- Assume $\|\Phi(x_n)\| \leqslant r$ and $|y_n - \langle \Phi(x_n), \theta_*\rangle| \leqslant \sigma$
- No assumption regarding lowest eigenvalues of the Hessian

$$\mathbb{E}\mathcal{R}(\bar{\theta}_n) - \mathcal{R}(\theta_*) \leqslant \frac{4\sigma^2 d}{n} + \frac{\|\theta_0 - \theta_*\|^2}{\gamma n}$$

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- Matches statistical lower bound (Tsybakov, 2003).
- Optimal rate with "large" step sizes

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Further references

Many stochastic algorithms not covered in this talk (coordinate descent, online Newton, composite optimization, non convex learning) ...

- Good introduction: Francis's lecture notes at Orsay
- Book:
  Convex Optimization: Algorithms and Complexity,
  Sébastien Bubeck

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