A quest for theoretically-sound optimization

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February 2024

“How did I get here?”-David Byrne

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JAMES MADISON UNIVERSITY

NC STATE UNIVERSITY

TU berlin + ZIB ZUSE INSTITUTE BERLIN

Lise
6.05 – 8 petaflop/second
(roughly 75 – 100 IBM Watsons)

Theoretically-sound optimization

What is optimization?

Optimization in a nutshell ($\mathcal{H} = \mathbb{R}^n$ or any real Hilbert space)

- **Objective function** $f : \mathcal{H} \to \mathbb{R} \cup \{+\infty\}$.

  e.g., data fidelity in ML, energy efficiency, profit, statistical error, . . .

- An "optimal" $x \in \mathcal{H}$ makes $f(x)$ the smallest or largest

  e.g., minimize error, maximize efficiency

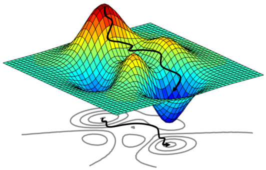


image: towardsdatascience.com

$$\underset{x \in \mathcal{H}}{\text{minimize}} \;\; f(x)$$

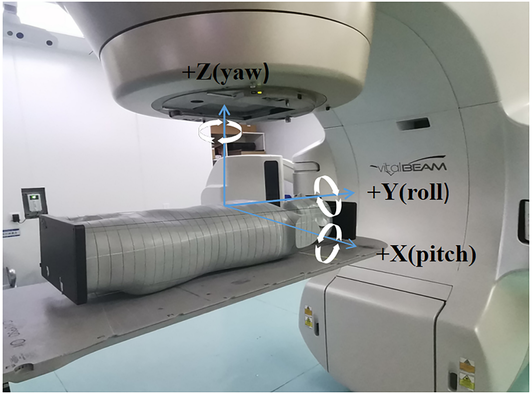
Constraint set(s) $C \subset \mathcal{H}$

e.g., $\mathbb{R}^N_+$, $\mathbb{S}^N_+$, hypercube, solution set of an inverse problem, . . .

$$\iota_C(x) = \begin{cases} 0 & \text{if } \; x \in C \\ +\infty & \text{otherwise.} \end{cases}$$

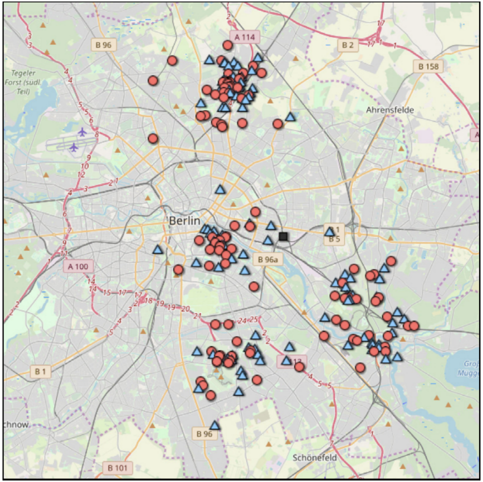
$$\underset{x \in C}{\text{minimize}} \;\; \widetilde{f}(x) = \underset{x \in \mathcal{H}}{\text{minimize}} \;\; \underbrace{\widetilde{f}(x) + \iota_C(x)}_{f}$$

Modeling via optimization



[Torelli et al., *Med. Phys.*, 2023]

image: [Fu et al., *Tech. Cancer Res. Treatment*, 2023]



[Sartori & Buriol, *Comput. Oper. Res.*, 2020]

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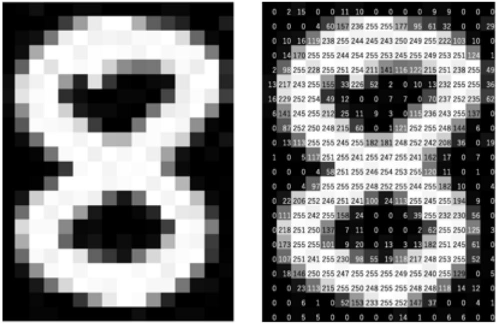

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0	10	16	119	238	255	244	245	243	250	249	255	222	103	10	0
0	14	170	255	255	244	254	255	253	245	255	249	253	251	124	1
2	98	255	228	255	251	254	211	141	116	122	215	251	238	255	49
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16	229	252	254	49	12	0	0	7	7	0	70	237	252	235	62
6	141	245	255	212	25	11	9	3	0	115	236	243	255	137	0
0	87	252	250	248	215	60	0	1	121	252	255	248	144	6	0
0	13	113	255	255	245	255	182	181	248	252	242	208	36	0	19
1	0	5	117	251	255	241	255	247	255	241	162	17	0	7	0
0	0	0	4	58	251	255	246	254	253	255	120	11	0	1	0
0	0	4	97	255	255	255	248	252	255	244	255	182	10	0	4
0	22	206	252	246	251	241	100	24	113	255	245	255	194	9	0
0	111	255	242	255	158	24	0	0	6	39	255	232	230	56	0
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0	173	255	255	101	9	20	0	13	3	13	182	251	245	61	0
0	107	251	241	255	230	98	55	19	118	217	248	253	255	52	4
0	18	146	250	255	247	255	255	255	249	255	240	255	129	0	5
0	0	23	113	215	255	250	248	255	255	248	248	118	14	12	0
0	0	6	1	0	52	153	233	255	252	147	37	0	0	4	1
0	0	5	5	0	0	0	0	0	14	1	0	6	6	0	0

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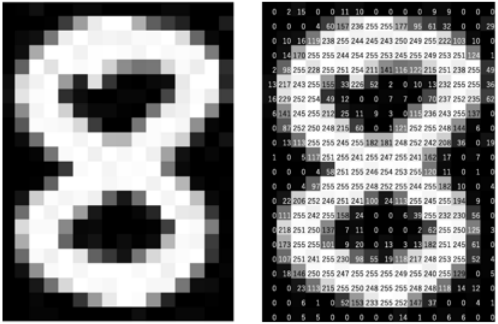

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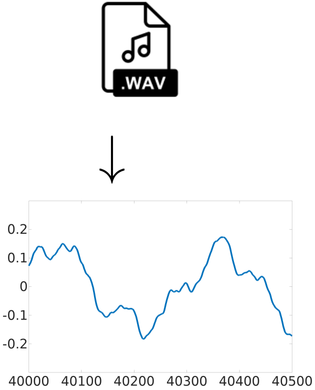
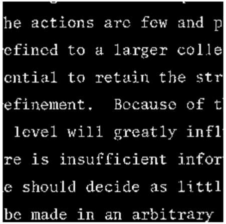
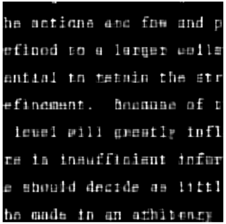


Modeling via optimization



Original

Observation

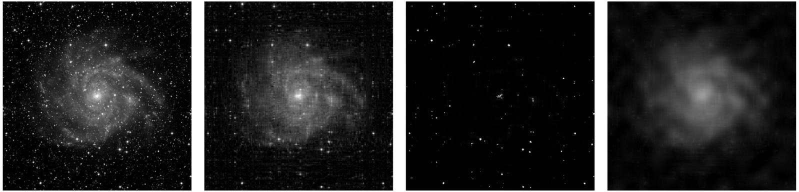


Recovery

[Combettes & ZW., *SIAM J. Imaging Sci.*, 2022]

Modeling via optimization

Original Observation Recovery



Original Observation Recovered stars Recovered galaxy

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Some fundamental questions

- What are the roadblocks to *provably* solving optimization problems?

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- What are the roadblocks to *provably* solving optimization problems?

  → Nonconvexity, nonsmoothness, and bears – oh my!

- What *theoretically-sound* algorithms exist, and can we do better?

  → Splitting, Parallelization, Extrapolation, Asynchronous computation

Theoretically-sound optimization

1. Motivation
2. Background: Theory vs practice
3. Proximity operators: Algorithmic bells and whistles
4. Splitting FW: What if the “usual” tools fail us?
5. More adventuring

Our setting

$\mathcal{H}$ is a real Hilbert space with inner product $\langle \cdot \mid \cdot \rangle$,
e.g., $\mathbb{R}^n$ with the dot product $\langle x \mid y \rangle = x^T y$.

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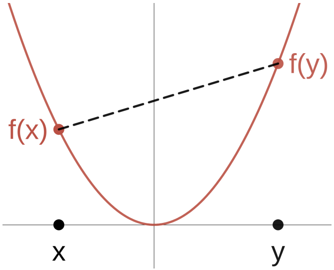

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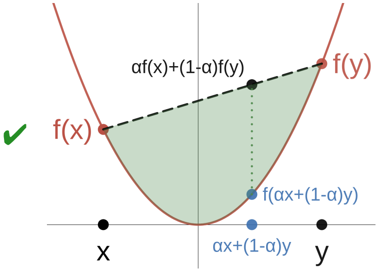

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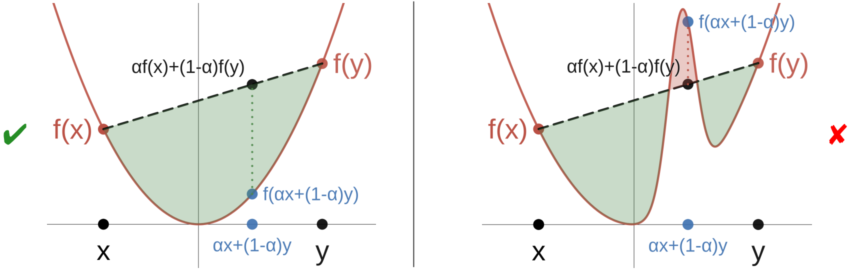

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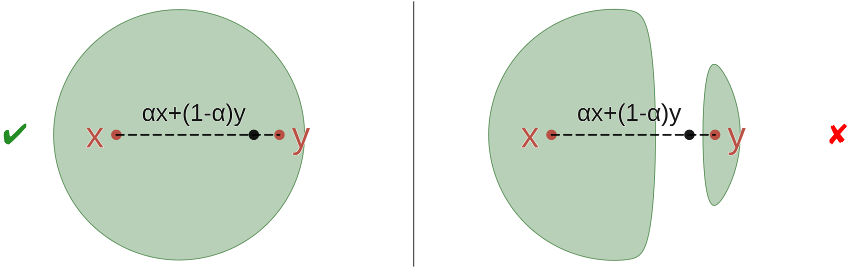

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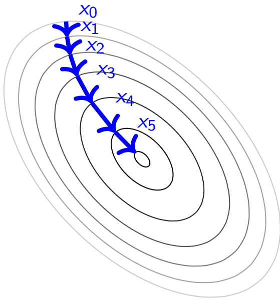
not $\|\mathcal{N}(x) - d\|$ for multilayer neural networks

"Traditioooon" -Tevye, Fiddler on the Roof

f is L-**smooth** $(L \geqslant 0)$ if it is differentiable and $\|\nabla f(x) - \nabla f(y)\| \leqslant L\|x - y\|$.



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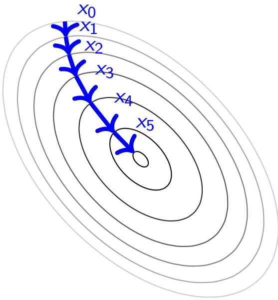
Gradient Descent

Let $f\colon \mathcal{H} \to \mathbb{R}$ be L-smooth and suppose $\operatorname{Argmin} f \neq \varnothing$. Let $x_0 \in \mathcal{H}$, $\varepsilon > 0$ and for every $n \in \mathbb{N}$, set

$$x_{n+1} = x_n - \lambda_n \nabla f(x_n), \qquad \text{where } \lambda_n \in \left[\varepsilon, \frac{2}{L} - \varepsilon\right] \tag{GD}$$

If $f \in \Gamma_0(\mathcal{H})$, then $(x_n)_{n\in\mathbb{N}}$ converges to a minimizer of f.



Foe #1: Non-convexity

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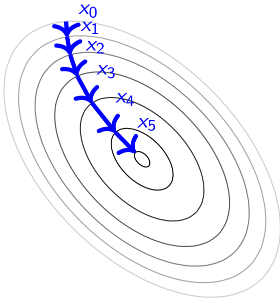
If $f \notin \Gamma_0(\mathcal{H})$, then $(x_n)_{n\in\mathbb{N}}$ coverges to a $\underbrace{\textbf{stationary point}}_{(\nabla f(x^*) = 0)}$.

For x_0 sufficiently close to a minimizer, $(x_n)_{n\in\mathbb{N}}$ converges to one.



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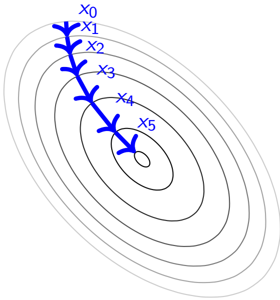

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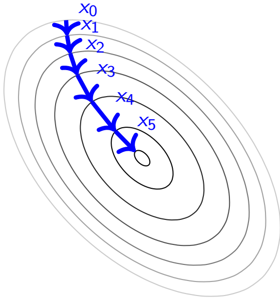
Stochastic Gradient Descent (one variant)

Let $f\colon \mathcal{H} \to \mathbb{R}$ be L-smooth and suppose $\operatorname{Argmin} f \neq \varnothing$. Let $x_0 \in \mathcal{H}$ and for every $n \in \mathbb{N}$, set

$$x_{n+1} = x_n - \frac{1}{n+1}\nabla f_{i_n}(x_n), \qquad \text{where } i_n \sim U(\{1, \dots, m\}) \quad \text{(SGD)}$$

If $f \in \Gamma_0(\mathcal{H})$, then $\mathbb{E}[f(x_n)]$ converges to $\inf_{x \in \mathcal{H}} f(x)$.



Why can't we take the eagles to Mordor?

(A reasonable question to ask, if we didn't read the books)

A common paradigm:

1. Define an objective function
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[Pontil et al., *Numer. Algorithms*, 2019]

Training a sparse linear binary classifier

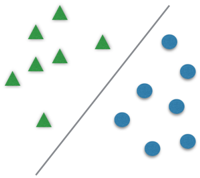

image: adeveloperdiary.com

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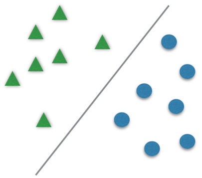

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$$\underset{x\in\mathbb{R}^n}{\text{minimize}} \sum_{i\in I_1} \max\{0, 1-\langle x \mid a_i\rangle\} + \sum_{i\in I_2} \max\{0, 1+\langle x \mid a_i\rangle\} + \lambda\|x\|_1$$

Foe #2: Non-differentiability

A common paradigm:

1. Define an objective function
2. Optimize with an efficient algorithm, e.g., SGD with algorithmic differentiation (AD)

Issue: For many objective functions, a gradient does not exist.

[Pontil et al., *Numer. Algorithms*, 2019]

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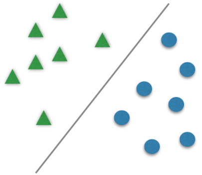

image: adeveloperdiary.com

$$\operatorname*{minimize}_{x\in\mathbb{R}^n} \sum_{i\in I_1} \max\{0, 1-\langle x \mid a_i\rangle\} + \sum_{i\in I_2} \max\{0, 1+\langle x \mid a_i\rangle\} + \lambda\|x\|_1$$

Foe #2: Non-differentiability

A common paradigm:

1. Define an objective function
2. Optimize with an efficient algorithm, e.g., SGD with algorithmic differentiation (AD)

Issue: For many objective functions, a gradient does not exist.

Engineers*:

image: ripleys.com

*:Some ~~mathematicians at heart~~ exceptions exist

How do we solve $\nabla f = 0$ when ∇f doesn't exist?

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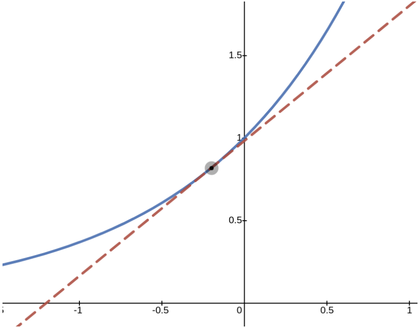
If $f \in \Gamma_0(\mathcal{H})$ is differentiable at $x \in \mathcal{H}$, then

$$(\forall y \in \mathcal{H}) \qquad \left\langle y - x \,\middle|\, \nabla f(x) \right\rangle + f(x) \leqslant f(y).$$



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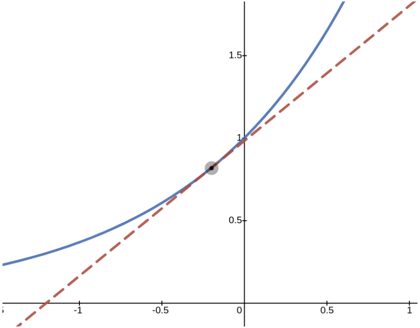

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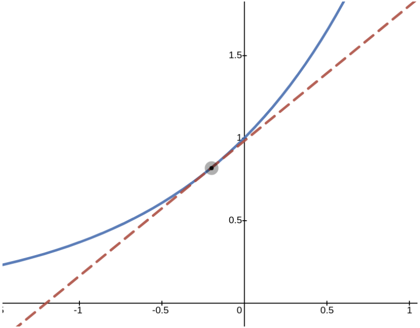

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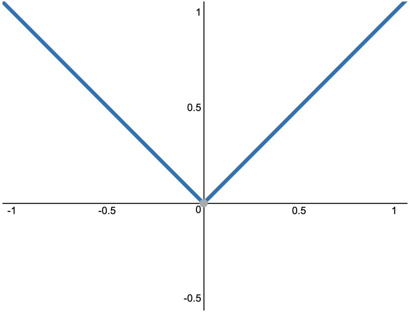

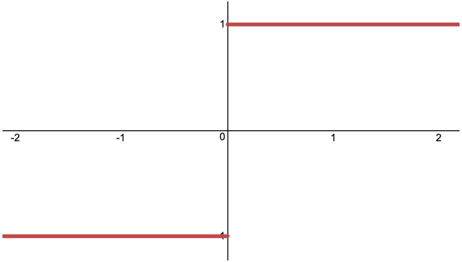

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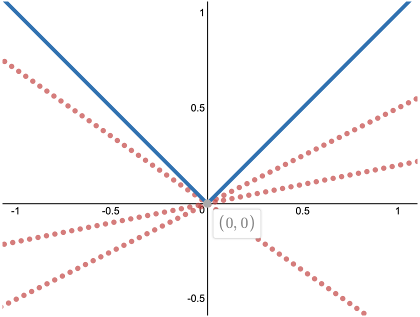

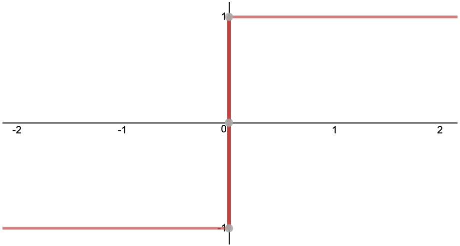

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Let $x \in \mathcal{H}$. Then $x \in \operatorname{Argmin} f$ if and only if $0 \in \partial f(x)$.

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Proof:

$$\begin{aligned} 0 \in \partial f(x) &\Leftrightarrow (\forall y \in \mathcal{H}) \quad \langle y - x | 0 \rangle + f(x) \leqslant f(y) \\ &\Leftrightarrow (\forall y \in \mathcal{H}) \quad f(x) \leqslant f(y) \\ &\Leftrightarrow x \in \operatorname{Argmin} \; f \end{aligned}$$

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∂f is useful for developing both $\underbrace{\text{optimality criterion}}_{0 \in \partial f(x)}$ and algorithms.

Goal: "$0 \in \partial f(x)$". Which path do we take?

image: centralldm.es

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Some *provenly-convergent* (first-order) algorithm classes:

- Subgradient-projections (e.g., in [C. & ZW, *IEEE EUSIPCO*, 2020])
- Proximity operators (e.g., in [C., B., & ZW, *IEEE ICASSP*, 2022], [C. & ZW, *J. Approx. Theory*, 2021], [C. & ZW, *SIAM J. Imaging Sci.*, 2023])
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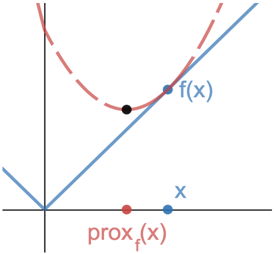
Theoretically-sound optimization

Proximity operators: a new hope

The **proximity operator of** f at $x \in \mathcal{H}$ is

$$\operatorname{prox}_f(x) = \underset{u \in \mathcal{H}}{\operatorname{Argmin}} \; f(u) + \frac{1}{2}\|x - u\|^2$$



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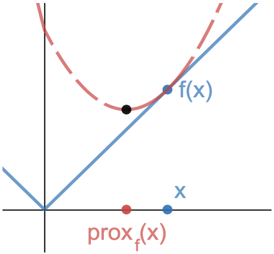

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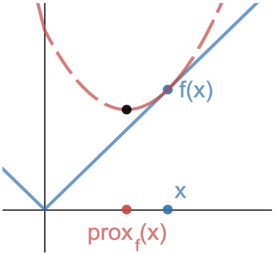

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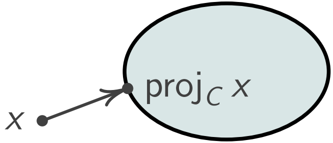

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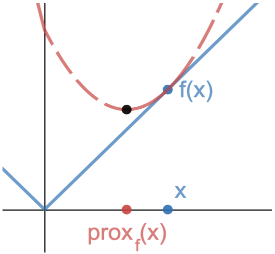

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$$x_{n+1} = \operatorname{prox}_{\gamma f} x_n.$$

Then $(x_n)_{n \in \mathbb{N}} \rightharpoonup x^* \in \operatorname{Argmin} f$.

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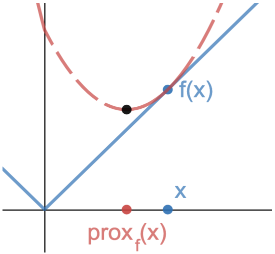

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Evolution of prox-based algorithms

$$f = \sum_{1 \leqslant i \leqslant m} f_i$$

$(\text{prox}_{f_i})_{1 \leqslant i \leqslant m}$ are simpler than prox_f.

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Open-source repo's:

Python/Matlab:
`proximity-operator.net`,

Julia:
`ProximalOperators.jl` (Github)

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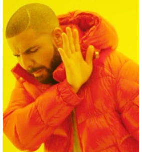
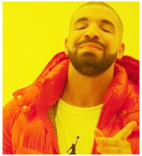
Algorithmic “Splitting” mentality:

	prox_f
	$\mathrm{prox}_{f_1}, \ldots \mathrm{prox}_{f_m}$

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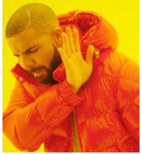

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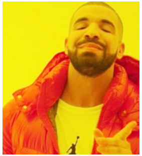

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Pseudocode for many proximal splitting algorithms*

Require: Point $x_0 \in \mathcal{H}$, objective function f

for $n = 0, 1$ **to** $\ldots$ **do**
  \# Preprocess x_n
  for $i = 1$ **to** m **do**
    $y_{i,n+1} \leftarrow$ evaluation of $\mathrm{prox}_{f_i}(\cdot)$
  end for
  $x_{n+1} \leftarrow$ combine $(y_{i,n+1})_{1 \leqslant i \leqslant m}$
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*:e.g., Douglas-Rachford, ADMM, Chambolle-Pock, Forward-backward, Augmented Lagrangian, ...

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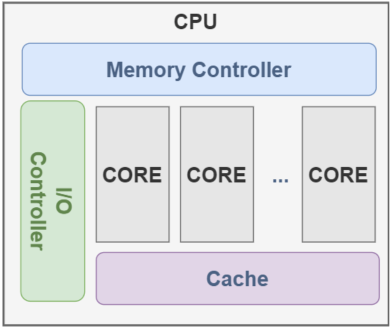

image: baeldung.com

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Require: Point $x_0 \in \mathcal{H}$, objective function f

```
for n = 0, 1 to ... do
    # Preprocess x_n
    for i = 1 to m do
        y_{i,n+1} ← evaluation of prox_{f_i}(·)
    end for
    x_{n+1} ← combine (y_{i,n+1})_{1≤i≤m}
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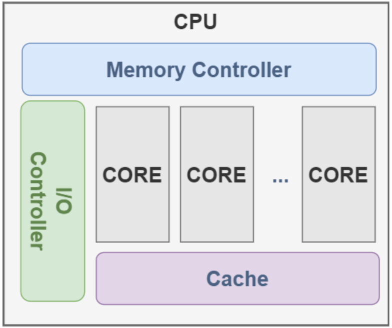

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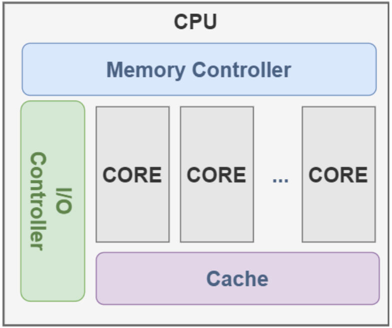

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Pseudocode for block-iterative proximal splitting algorithms

Require: Point $x_0 \in \mathcal{H}$, objective function f

for $n = 0, 1$ **to** $\ldots$ **do**

  \# Preprocess x_n; Select $I_n \subset \{1, \ldots, m\}$

  for $i = 1$ **to** m **do**

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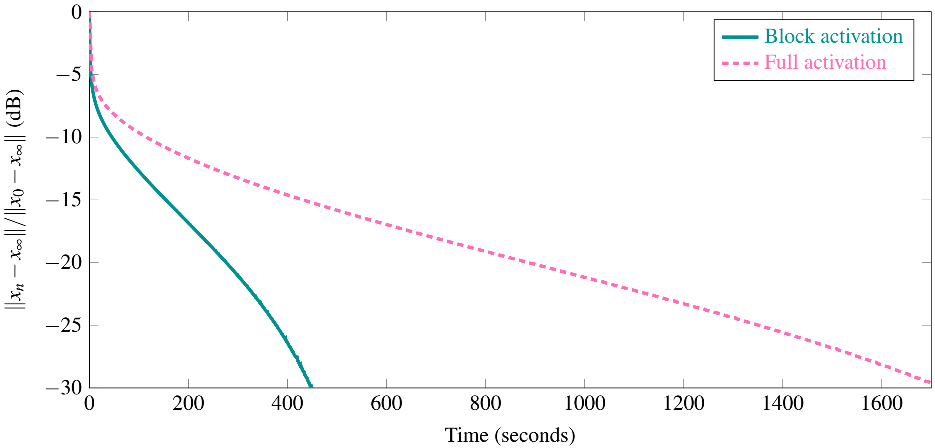
Block activation for image recovery ($m = 2$)



[C. & ZW, *SIAM J. Imaging Sci.*, 2022] Relative error for full-activation ($I_n = I$) versus block activation:

$$I_n = \begin{cases} \{1,2\}, & \text{if } n \equiv 0 \mod 5; \\ \{2\}, & \text{if } n \not\equiv 0 \mod 5. \end{cases}$$

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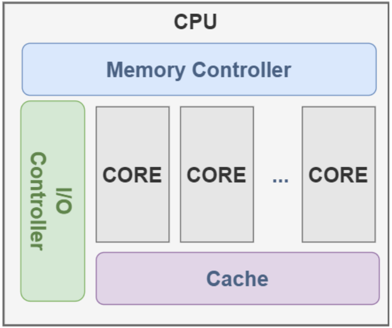

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Two (currently separate) approaches:

→ Asynchronous updates

→ Extrapolated updates

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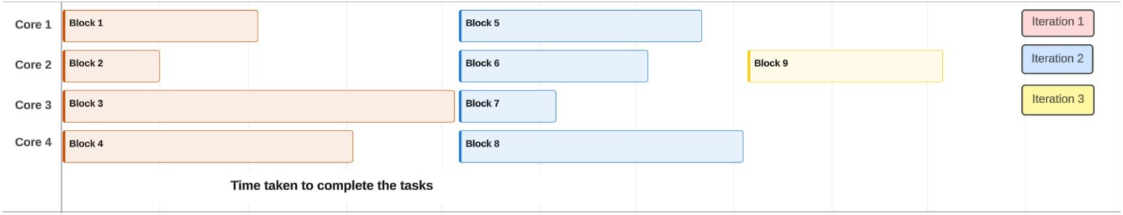
Evolution of prox-based algorithms

Parallel and Synchronous



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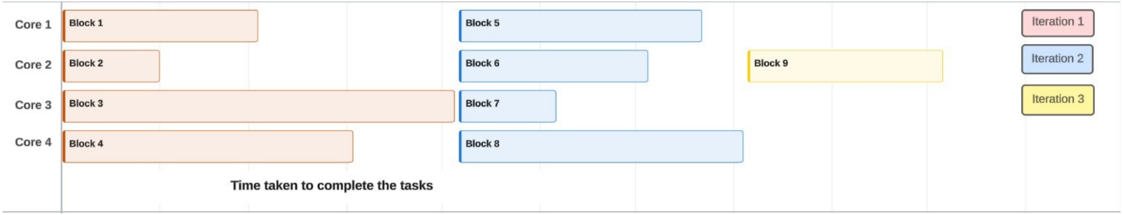
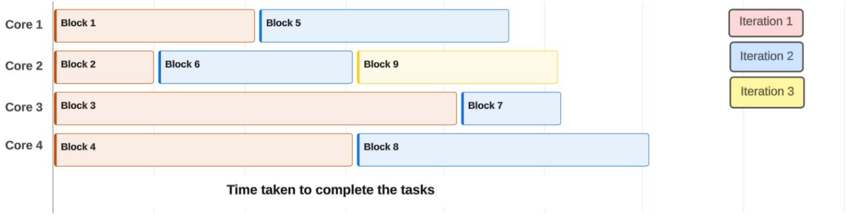


Parallel and **Asynchronous**



Asynchrony: Projective Splitting Algorithms

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Only studied **synchronous** case!

Asynchrony: Projective Splitting Algorithms

[Eckstein & Svaiter, *Math Prog. A*, 2008]:

Coined "Projective splitting" (synchronous, not block-iterative).
[Combettes & Eckstein, *Math Prog. B*, 2018]:

Convergence proof with **asynchronous block-iterative** updates!

[Combettes, Búi, & ZW, *IEEE ICASSP*, 2022]:

Numerical analysis (space and time complexity). For ML (training classifiers) and image processing, works better than other algorithms in its class.
Only studied **synchronous** case!

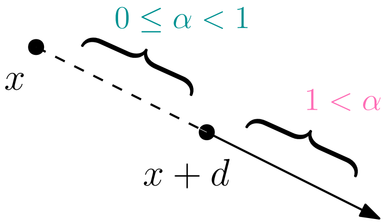
Dua, Goel, Sharma, & ZW (ongoing work):

Analysis and experimentation for **asynchronous** case. `AsyncProx.jl` in development.

Over-relaxation (extrapolation)

Given a "descent direction" d (e.g., combination of $(y_{i,n+1})_{1\leqslant i\leqslant m}$) from $x \in \mathcal{H}$,

$$x_+ = (1-\alpha)x + \alpha(x+d)$$



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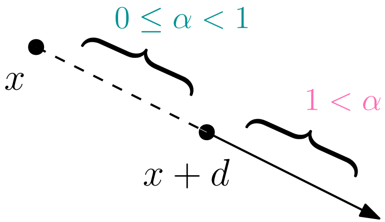
$0 \leqslant \alpha < 1$: under-relaxation

$1 < \alpha$: over-relaxation



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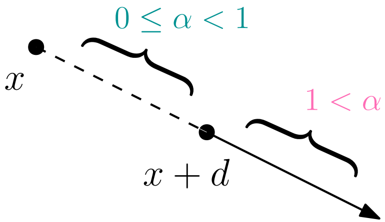
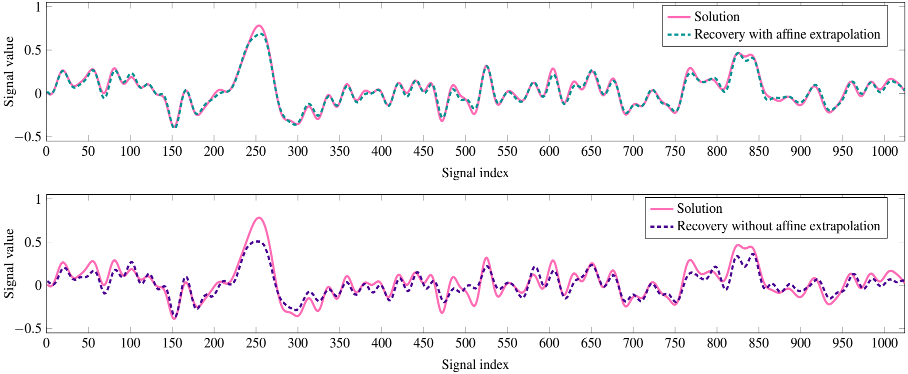


$$x_{n+1} = x_n - \alpha_n \frac{1}{L}\nabla f(x_n), \qquad \text{where } \alpha_n \in [\varepsilon, 2-\varepsilon] \tag{GD}$$
$$= (1-\alpha_n)x_n + \alpha_n \left(x_n - \frac{1}{L}\nabla f(x_n)\right)$$

Over-relaxation for fixed-point problems

[Combettes & ZW, *J. Approx. Theory*, 2021]:
A strongly-convergent algorithm with affine-convex extrapolation.
Example: EEG data (minimal-norm solution to an ill-posed nonlinear inverse problem; recovery after 1000 iterations, < 1 minute.)



Theoretically-sound optimization

1. Motivation
2. Background: Theory vs practice
3. Proximity operators: Algorithmic bells and whistles
4. Splitting FW: What if the “usual” tools fail us?
5. More adventuring

They stole my horse!

Splitting problem setup

Given a smooth function $f:\mathbb{R}^n \to \mathbb{R}$ and compact convex sets $(C_i)_{1\leqslant i\leqslant m}$

$$\text{minimize} \quad f(x) \quad \text{subject to} \quad x \in \bigcap_{1\leqslant i\leqslant m} C_i, \tag{$\star$}$$

Applications: data science, matrix decomposition, quantum computing, combinatorial graph theory

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What if $(\mathrm{proj}_{C_i})_{1 \leqslant i \leqslant m}$ are too expensive? $\leftarrow$ e.g., in high-dimensional settings!

A spark of inspiration

Frank-Wolfe / "Conditional gradient" alg. [Naval Res. Logist. Quart., 1956]

Given a smooth function $f\colon \mathbb{R}^n \to \mathbb{R}$ and a nonempty compact convex set C,

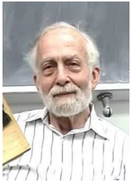
$$\text{minimize} \;\; f(x) \;\; \text{subject to} \;\; x \in C$$

Instead of projecting, use a *linear minimization oracle* of C,

$$\mathrm{LMO}_C\colon y \mapsto p \in \operatorname{Argmin}_{x\in C} \langle y \mid x \rangle \tag{LMO}$$

$$x_{n+1} = x_n + \frac{1}{n+1}\Big(\mathrm{LMO}_C(\nabla f(x_n)) - x_n\Big)$$

Marguerite Frank



Philip Wolfe

efficiency(LMOs) == efficiency(lembus bread)

[Combettes/Pokutta, '21]: For many $\underbrace{\text{constraints}}$, C, proj_C is **more expensive** than LMO_C.
(e.g., nuclear norm ball, ℓ_1 ball, probability simplex, Birkhoff polytope, general LP, ...)

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Example: Nuclear norm ball

For $x \in \mathbb{R}^{n\times n}$

$$\|x\|_{nuc} = \sum_{1\leqslant i\leqslant n} \sigma_i(x).$$

For $\beta \geqslant 0$, $C = \{x \in \mathbb{R}^{n\times n} \mid \|x\|_{nuc} \leqslant \beta\}$,

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$\text{proj}_C(x)$: requires a full SVD!
$(\sigma_1, \ldots, \sigma_n, U, V)$, where $x = U \text{diag}(\sigma_1, \ldots, \sigma_n) V^\top$

Full SVD

$n = 500$: `0.11 sec`

$n = 1000$: `0.47 sec`

$n = 2000$: `4.87 sec`

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$\text{LMO}_C(x)$: requires only first singular value/vectors
$(\sigma_1, U_1, V_1^\top)$

Full SVD

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$n = 1000$: `0.47 sec`

$n = 2000$: `4.87 sec`

Just $(\sigma_1, U_1, V_1^\top)$

$n = 500$: `0.0081 sec`

$n = 1000$: `0.056 sec`

$n = 2000$: `0.638 sec`

Sure would be nice if we could use splitting...

$$\text{minimize } f(x) \text{ subject to } x \in \bigcap_{1 \leqslant i \leqslant m} C_i, \tag{$\star$}$$

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LMO-based *splitting algorithms*, enforce constraints via LMOs for the individual sets

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$\rightarrow$ Unlike projections, LMOs are discontinuous.

$\rightarrow$ "State-of-the-art" relies on inexact prox-based algorithms.

It's aliiive!

[ZW & P, 2024]: Split Conditional Gradient Algorithm

Require: Point $x_0 \in \frac{1}{m}\sum_{1\leqslant i\leqslant m} C_i$, smooth function f

```
for t = 0, 1 to ... do
    Choose penalty parameter λ_t ∈ ]0, +∞[
    Choose step size γ_t ∈ ]0, 1]
    g_t ← ∇f(x_t)
    for i = 1 to m do
        v_t^i ← LMO_{C_i}(g_t + λ_t(x_t^i − x_t))
        x_{t+1}^i ← x_t^i + γ_t(v_t^i − x_t^i)
    end for
    x_{t+1} ← (1/m) Σ_{1⩽i⩽m} x_{t+1}^i
end for
```

$$\begin{aligned}
&\textbf{for } t = 0, 1 \textbf{ to } \dots \textbf{ do}\\
&\quad \text{Choose penalty parameter } \lambda_t \in \,]0, +\infty[\\
&\quad \text{Choose step size } \gamma_t \in \,]0, 1]\\
&\quad g_t \leftarrow \nabla f(x_t)\\
&\quad \textbf{for } i = 1 \textbf{ to } m \textbf{ do}\\
&\quad\quad \boldsymbol{v}_t^i \leftarrow \mathrm{LMO}_{C_i}(g_t + \lambda_t(\boldsymbol{x}_t^i - x_t))\\
&\quad\quad \boldsymbol{x}_{t+1}^i \leftarrow \boldsymbol{x}_t^i + \gamma_t(\boldsymbol{v}_t^i - \boldsymbol{x}_t^i)\\
&\quad \textbf{end for}\\
&\quad x_{t+1} \leftarrow \frac{1}{m}\sum_{1\leqslant i\leqslant m} \boldsymbol{x}_{t+1}^i\\
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Practical advantages:

→ Uses individual LMOs

→ Lowest-known # LMO calls: one LMO per set (per iteration)

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Q: Does it actually solve $(\star)$?

A: Yes.

$\gamma_t = \mathcal{O}(1/\sqrt{t})$ and
$\lambda_t = \mathcal{O}(\ln t)$ work.
(whether or not f is convex).

Convergence

Theorem ([ZW & P., 2024])

Let f be L-smooth and let $(C_i)_{1\leqslant i\leqslant m}$ be nonempty compact convex subsets of $\mathcal{H}$ such that $\bigcap_{1\leqslant i\leqslant m} C_i \neq \varnothing$. Let $\lambda_0 > 0$ and $\lambda_{t+1} = \lambda_t + (\sqrt{t}+2)^{-2}$ and $\gamma_t = 2/(\sqrt{t}+2)$. If f is **convex**, then

$$f\left(\frac{1}{m}\sum_{1\leqslant i\leqslant m} \boldsymbol{x}_t^i\right) \to \inf_{x\in\bigcap_{1\leqslant i\leqslant m} C_i} f(x)$$

and every accumulation point $\boldsymbol{x}_\infty$ of $(\boldsymbol{x}_t)_{t\in\mathbb{N}}$ produces a solution $\frac{1}{m}\sum_{1\leqslant i\leqslant m} \boldsymbol{x}_\infty^i \in \bigcap_{1\leqslant i\leqslant m} C_i$ such that $f(\frac{1}{m}\sum_{1\leqslant i\leqslant m} \boldsymbol{x}_\infty) = \inf_{x\in\bigcap_{1\leqslant i\leqslant m} C_i} f(x)$.

Nonconvex convergence results too: arXiv:2311.05381

Theoretically-sound optimization

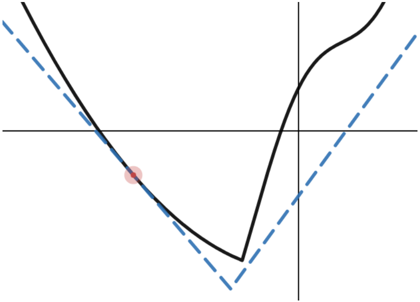
Abs-smooth optimization

Abs-smooth functions f include compositions of smooth functions, max, min, and $|\cdot|$. ...

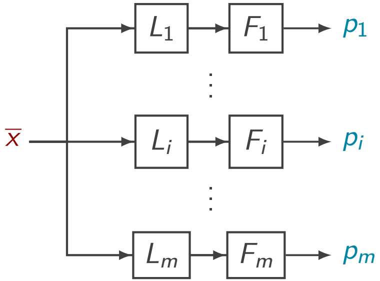
→ Loss functions for multilayer Neural Networks with smooth and/or ReLU activation.

→ Allows one to find a local minimizer on non-convex objective functions!

→ Future work: Improve scalability.



Nonlinear inverse problems

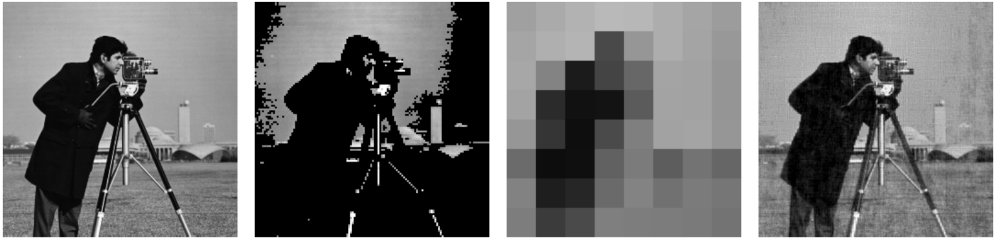


Given $(p_i)_{1 \leqslant i \leqslant m}$, find $x^* \in \mathcal{H}$ such that

$$(\forall i \in \{1, \dots, m\}) \quad F_i(L_i x^*) = p_i$$

L_i are bounded linear operators, and
$F_i \approx$ proximity operators.

$\rightarrow$ To-do: Stability analysis



Outlook and future work

- Improved convergence rates and acceleration
- Block-iterative Frank-Wolfe algorithms
- Efficient prox/ LMO algorithms
- ...

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- Improved convergence rates and acceleration
- Block-iterative Frank-Wolfe algorithms
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- . . .

Potential collaborators: Hala Nelson, Minah Oh, Roger Thelwell, and more!

For students:

Proofs (MATH 245), sequences and series (236), gradients (237), linear algebra (238/300/434), optimization theory (340), coding experience (248/250/448/449), analysis (410/411).

REUs & Grad School in Berlin: `iol.zib.de` (Opt/ML), `math-berlin.de`

Thank you for your attention!

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Supplement

$$f = \sum_{1 \leqslant i \leqslant m} f_i$$

$(\mathrm{prox}_{f_i})_{1 \leqslant i \leqslant m}$ are simpler than prox_f.

e.g., $\boxed{\text{Find } x \in \mathbb{S}^n_+ \cap [\alpha, \beta]^{N \times N}}$

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \ \iota_{\mathbb{S}^n_+}(x) + \iota_{[\alpha,\beta]^N}(x)$$

prox_f is intractable.

$$\left.\begin{aligned} \mathrm{prox}_{f_1} &= \mathrm{proj}_{[\alpha,\beta]^N} \\ \mathrm{prox}_{f_2} &= \mathrm{proj}_{\mathbb{S}^n_+} \end{aligned}\right\} \text{known in closed-form.}$$