Performance Estimation Problems (PEPs):

Tutorial – Session 3/3

Aymeric Dieuleveut, Adrien Taylor





SMAI-MODE tutorial – March 2026

Designing algorithms

A "generic" first-order method

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\begin{aligned}
w_1 &= w_0 - \alpha_{1,0}\nabla f(w_0) \\
w_2 &= w_1 - \alpha_{2,0}\nabla f(w_0) - \alpha_{2,1}\nabla f(w_1) \\
w_3 &= w_2 - \alpha_{3,0}\nabla f(w_0) - \alpha_{3,1}\nabla f(w_1) - \alpha_{3,2}\nabla f(w_2) \\
&\vdots \\
w_n &= w_{n-1} - \sum_{i=0}^{n-1} \alpha_{n,i}\nabla f(w_i),
\end{aligned}
\tag{FOM}
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for some coefficients $\{\alpha_{i,j}\}$. Generic **non-adaptive** first-order method.

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How to choose $\{\alpha_{i,j}\}$?

- ◇ pick a performance criterion, for instance $\frac{\|w_n - w_\star\|^2}{\|w_0 - w_\star\|^2}$,
- ◇ solve the minimax (minimize worst-case): $\min_{\{\alpha_{i,j}\}_{i,j}} \max_{f\in\mathcal{F},\{w_i\}} \frac{\|w_n - w_\star\|^2}{\|w_0 - w_\star\|^2}$.

Traditional design

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- ◇ unconstrained quadratic programming:

  first-order methods $\Leftrightarrow$ polynomials $\rightarrow$ optimal algorithms via optimal polynomials.[1,2,3]

[1] Golub and Varga (1961). "Chebyshev semi-iterative methods, successive overrelaxation iterative methods, and second order Richardson iterative methods." Numerische Mathematik.

[2] Polyak (1987). "Introduction to optimization." Optimization Software.

[3] Nemirovski (1995). "Information-based complexity of convex programming." (Lecture notes)

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Algorithm design (with guarantees):

- ◇ unconstrained quadratic programming:

  first-order methods $\Leftrightarrow$ polynomials $\rightarrow$ optimal algorithms via optimal polynomials.[1,2,3]

- ◇ Beyond quadratics: traditionally more "hand-crafted"
  - – Analogy with conjugate gradients.[4,5]
  - – Lyapunov function-type analyses.[6,7]

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[4] Nemirovski (1982). "Orth-method for smooth convex optimization." (in Russian) Engineering Cybernetics.

[5] Narkiss and Zibulevsky (2005). "Sequential subspace optimization method for large-scale unconstrained problems."

[6] Nesterov (1983). "A method for solving the convex programming problem with convergence rate $O(1/k^2)$." Dokl. akad. nauk. Sssr 269.

[7] Beck and Teboulle (2009). "A fast iterative shrinkage-thresholding algorithm for linear inverse problems." SIAM journal on imaging sciences 2(1).

Design problem

How to solve the design problem (or proxy of it)?

$$\min_{\{\alpha_{i,j}\}} \max_{f \in \mathcal{F}} \frac{\|w_n - w_\star\|^2}{\|w_0 - w_\star\|^2} ?$$

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- ◇ analogies (e.g., with conjugate gradient methods)

$$w_{k+1} \in \operatorname*{argmin}_{x \in \mathbb{R}^d} \{f(w) : \ w \in w_0 + \operatorname{span}\{\nabla f(w_0), \ldots, \nabla f(w_k)\}\},$$

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- ◇ brutal approaches.

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Recall primal problem, with step-size optimization

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\min_{\alpha_{1,0}} \max_{G,\, F} \quad & G_{1,1} + \alpha_{1,0}^2 G_{2,2} - 2\alpha_{1,0} G_{1,2} \\
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Dualize inner maximization $\rightarrow$ min min.

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if $C \succ 0$: $M \succcurlyeq 0 \Leftrightarrow A - BC^{-1}B^T \succcurlyeq 0$

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When $N = 2$, the problem becomes

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for some $S_{1,1}, S_{1,2}, \ldots, S_{3,3}$ (functions of $\tau, \lambda_1, \ldots, \lambda_6$ and $\{\alpha_{i,j}\}$).

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In particular

$$S_{1,2} = -\frac{L\lambda_3 - 2(L-\mu)\alpha_{2,0} + \mu\lambda_1 + L\mu(\lambda_2+\lambda_5)\alpha_{1,0}}{L-\mu}$$
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LMI convex in some step-sizes ($\alpha_{2,0}$ and $\alpha_{2,1}$) but not in the others.

Forewords and problem statement

Numerical examples

Design via idealized algorithms

Concluding remarks

Numerical examples I

Example for $L = 1$ and $\mu = .1$

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$$[\alpha_{i,j}^\star] = \begin{bmatrix} 1.8182 \end{bmatrix}.$$

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- For $n = 4$, we reach $\frac{\|w_4 - w_\star\|^2}{\|w_0 - w_\star\|^2} \leqslant 0.0944$ with

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Numerical examples II

What about different performance measure? Example $\frac{f(w_n)-f_\star}{f(w_0)-f_\star}$ and $L = 1$, $\mu = .1$.

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$$[\alpha_{i,j}] = \begin{bmatrix} 1.9470 & & \\ 0.4599 & 2.2406 & \\ 0.1705 & 0.4599 & 1.9470 \end{bmatrix}.$$

- For $n = 4$, we obtain $\frac{f(w_4)-f_\star}{f(w_0)-f_\star} \leqslant 0.0789$ with

$$[\alpha_{i,j}] = \begin{bmatrix} 1.9187 & & & \\ 0.4098 & 2.1746 & & \\ 0.1796 & 0.5147 & 2.1746 & \\ 0.0627 & 0.1796 & 0.4098 & 1.9187 \end{bmatrix}.$$

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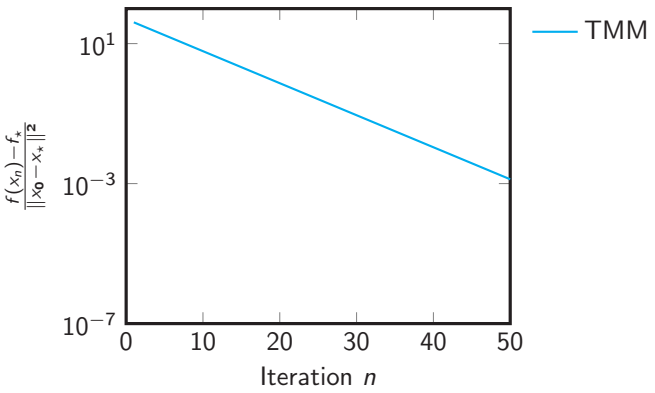

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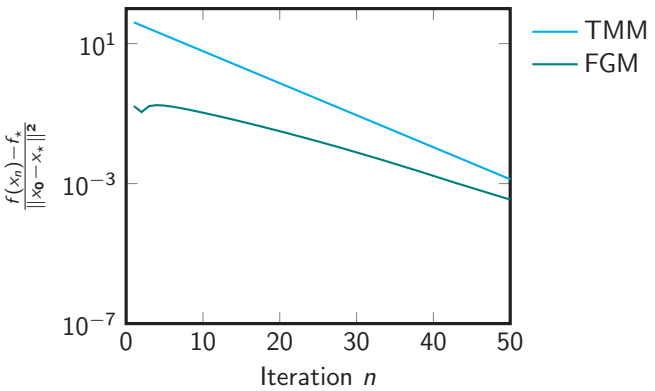

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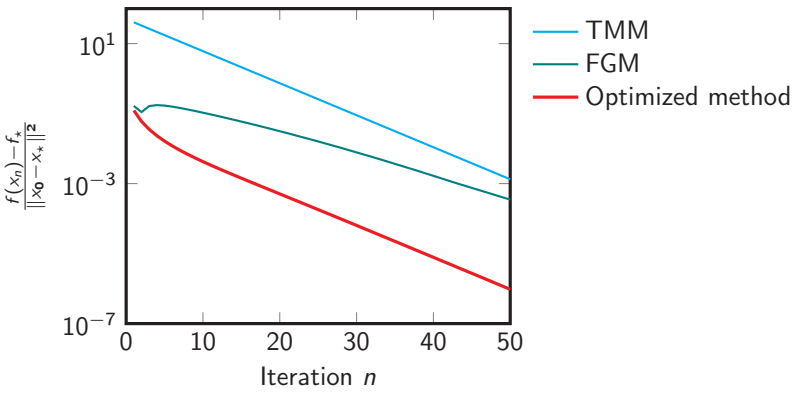

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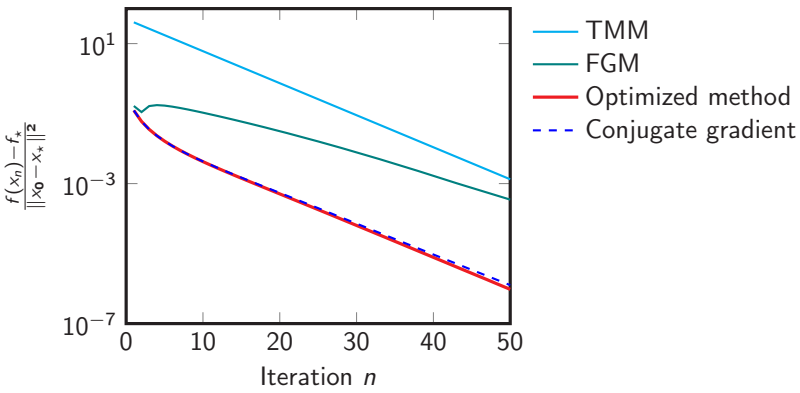

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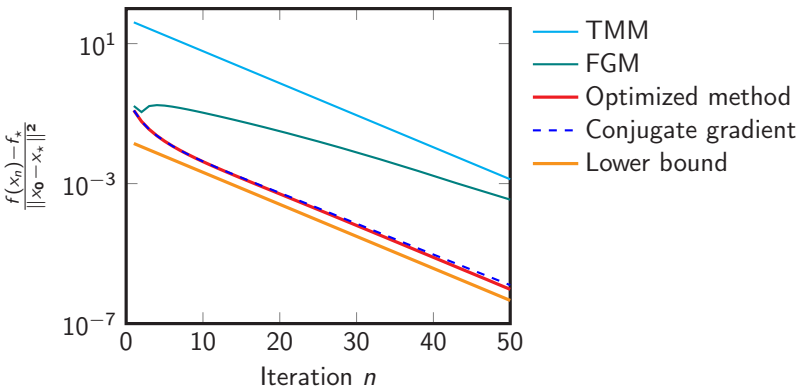

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- ◇ Beyond that, a few criterion/settings/methods for which "perfectly optimal" algorithms might be known, but matching lower bounds are still missing.
  - $\frac{\|\nabla f(w_n)\|^2}{f(w_0)-f_\star}$,[11]
  - a few numerically-generated methods, proximal variants, etc.

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Optimized gradient method (OGM)

Example I: the optimal method for $\frac{f(y_n)-f_\star}{\|y_0-y_\star\|^2}$ is called the "optimized gradient method".[12]

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Example I: the optimal method for $\frac{f(y_n)-f_\star}{\|y_0-y_\star\|^2}$ is called the "optimized gradient method".[12]

$$y_k = \tfrac{1}{\theta_k} z_k + \left(1 - \tfrac{1}{\theta_k}\right)\left(y_{k-1} - \tfrac{1}{L}\nabla f(y_{k-1})\right)$$
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which rely on some exotic sequence

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where $\theta_{-1} = 0$, and roughly $\theta_k \approx \frac{k}{2}$.

The (tight) worst-case guarantee: $\frac{f(y_n)-f_\star}{L\|y_0-y_\star\|^2} \leqslant \frac{1}{2\theta_n^2} \approx \frac{2}{n^2}$. Matches exactly lower bound.[13]

[12] Kim, Fessler (2016). "Optimized methods for smooth convex optimization."

[13] Drori (2017). "The exact information-based complexity of smooth convex minimization."

Information-Theoretic Exact Method (ITEM)

Example II: optimal method for $\frac{\|z_n - z_\star\|^2}{\|z_0 - z_\star\|^2}$ is "Information-Theoretic Exact Method":[14]

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Example II: optimal method for $\frac{\|z_n - z_\star\|^2}{\|z_0 - z_\star\|^2}$ is "Information-Theoretic Exact Method":[14]

$$y_k = (1-\beta_k)z_k + \beta_k\left(y_{k-1} - \frac{1}{L}\nabla f(y_{k-1})\right)$$
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where the sequences $\{\beta_k\}$ and $\{\delta_k\}$ depends on some external sequence $\{A_k\}$ with $A_k \geqslant \left(1-\sqrt{\frac{\mu}{L}}\right)^{-2k}$.

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The (tight) guarantee is $\frac{\|z_n - z_\star\|^2}{\|z_0 - z_\star\|^2} \leqslant \frac{1}{1+\frac{\mu}{L}A_n} = O\left(\left(1-\sqrt{\frac{\mu}{L}}\right)^{2n}\right)$. Matches exact lower bound.[15]

[14] T, Drori (2023). "An optimal gradient method for smooth strongly convex minimization."

[15] Drori, T (2022). "On the oracle complexity of smooth strongly convex minimization."

A few instructive examples

Design first-order methods via PEPs:

- Drori, Teboulle (2014). "Performance of first-order methods for smooth convex minimization: a novel approach." Mathematical Programming 145(1).
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... including "brutal" examples:

- ◇ Grimmer (2024). "Provably faster gradient descent via long steps." SIAM Journal on Optimization 34(3).
- ◇ Gupta, Van Parijs, Ryu (2024). "Branch-and-Bound Performance Estimation Programming: A Unified Methodology for Constructing Optimal Methods." Mathematical Programming 204(1).

Forewords and problem statement

Numerical examples

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Concluding remarks

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Let's exemplify:

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So, for any pair $\lambda_1, \lambda_2 \in \mathbb{R}$ we get:

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$$\rho \overset{\text{(def)}}{=} \max_{w_{\mathbf{0}}, w_{\mathbf{1}}, f \in \mathcal{F}_{\mu,\mathrm{L}}} \frac{f(w_1) - f_\star}{f(w_0) - f_\star} \text{ s.t. } \langle \nabla f(w_1), \nabla f(w_0) \rangle = 0, \ \langle \nabla f(w_1), w_1 - w_0 \rangle = 0,$$

upper bound from a Lagrangian relaxation with $\lambda_1, \lambda_2 \in \mathbb{R}$:

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We can also create an intermediary problem

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Bonus: there exists a choice $\lambda_1^\star, \lambda_2^\star$ such that

$$\rho = \bar{\rho}(\lambda_1^\star, \lambda_2^\star).$$

Design procedure

Algorithm constraints, and associated Lagrange multipliers:

$$\langle \nabla f(w_i), \nabla f(w_j) \rangle = 0, \qquad \text{for all } 0 \leqslant j < i = 1, \dots n \qquad : \beta_{i,j},$$
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benefits from the same worst-case convergence rate $\bar{\rho}$.

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Smooth convex minimization setting:

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

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Lower bound for large-scale setting ($d \geqslant n+2$) by Drori (2017):

$$f(x_n) - f(x_\star) \geqslant \frac{L\|x_0 - x_\star\|^2}{2\theta_n^2},$$

with $\theta_0 = 1$, and:

$$\theta_{i+1} = \begin{cases} \frac{1+\sqrt{4\theta_i^2+1}}{2} & \text{if } i \leqslant n-2, \\ \frac{1+\sqrt{8\theta_i^2+1}}{2} & \text{if } i = n-1. \end{cases}$$

As a result from subspace-search elimination, all methods satisfying (for $i = 1, \dots, n$)

$$\langle \nabla f(x_i); x_i - \left[\left(1 - \frac{1}{\theta_i}\right) \left(x_{i-1} - \tfrac{1}{L} \nabla f(x_{i-1})\right) + \frac{1}{\theta_i} \left(x_0 - \tfrac{2}{L} \sum_{j=0}^{i-1} \theta_j \nabla f(x_j) \right) \right] \rangle \leqslant 0$$

benefit from the same guarantee:

$$f(x_n) - f(x_\star) \leqslant \frac{L \|x_0 - x_\star\|^2}{2\theta_n^2},$$

Greedy First-order Method (GFOM)

Inputs: f, x_0, n.

For $i = 1, 2, \ldots, n$

$$x_{i+1} = \operatorname*{argmin}_{x \in \mathbb{R}^d} \{f(x) : \; x \in x_0 + \operatorname{span}\{\nabla f(x_0), \ldots, \nabla f(x_{i-1})\}\}.$$

Worst-case guarantee:

$$f(x_n) - f(x_\star) \leqslant \frac{L\|x_0 - x_\star\|^2}{2\theta_n^2}.$$

Optimized gradient methods

Three methods with the same (optimal) worst-case behavior

Optimized gradient method with exact line-search

Inputs: f, x_0, n.

For $i = 1, \ldots, n$

$$y_i = \left(1 - \frac{1}{\theta_i}\right) x_{i-1} + \frac{1}{\theta_i} x_0$$

$$d_i = \left(1 - \frac{1}{\theta_i}\right) \nabla f(x_{i-1}) + \frac{1}{\theta_i} \left(2 \sum_{j=0}^{i-1} \theta_j \nabla f(x_j)\right)$$

$$\alpha = \operatorname*{argmin}_{\alpha \in \mathbb{R}} f(y_i + \alpha d_i)$$

$$x_i = y_i + \alpha d_i$$

Worst-case guarantee: $f(x_n) - f(x_\star) \leqslant \frac{L\|x_0 - x_\star\|^2}{2\theta_n^2}$

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Optimized gradient method

Inputs: f, x_0, n.

For $i = 1, \dots, n$

$$y_i = x_{i-1} - \frac{1}{L}\nabla f(x_{i-1})$$

$$z_i = x_0 - \frac{2}{L}\sum_{j=0}^{i-1} \theta_j \nabla f(x_j)$$

$$x_i = \left(1 - \frac{1}{\theta_i}\right) y_i + \frac{1}{\theta_i} z_i$$

Worst-case guarantee: $f(x_n) - f(x_\star) \leqslant \frac{L\|x_0 - x_\star\|^2}{2\theta_n^2}$.

Forewords and problem statement

Numerical examples

Design via idealized algorithms

Concluding remarks

Feedback and challenging questions to the others

https://forms.gle/r5sPXw7ak1wXM3ie6

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- ◇ algebraic insights into performance analyses:
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  - – analyses are linear combinations of certain specific inequalities.

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  - – analyses are linear combinations of certain specific inequalities.

Byproducts:

- ◇ computer-assisted design of analyses,
- ◇ computer-assisted design of numerical methods,
- ◇ step towards reproducible theory
  - – validation & benchmark tool for proofs (also for reviews ☺).

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Acceleration/optimal methods by optimizing worst-cases.