

Mini-course on Sparse estimation off-the-grid Algorithms

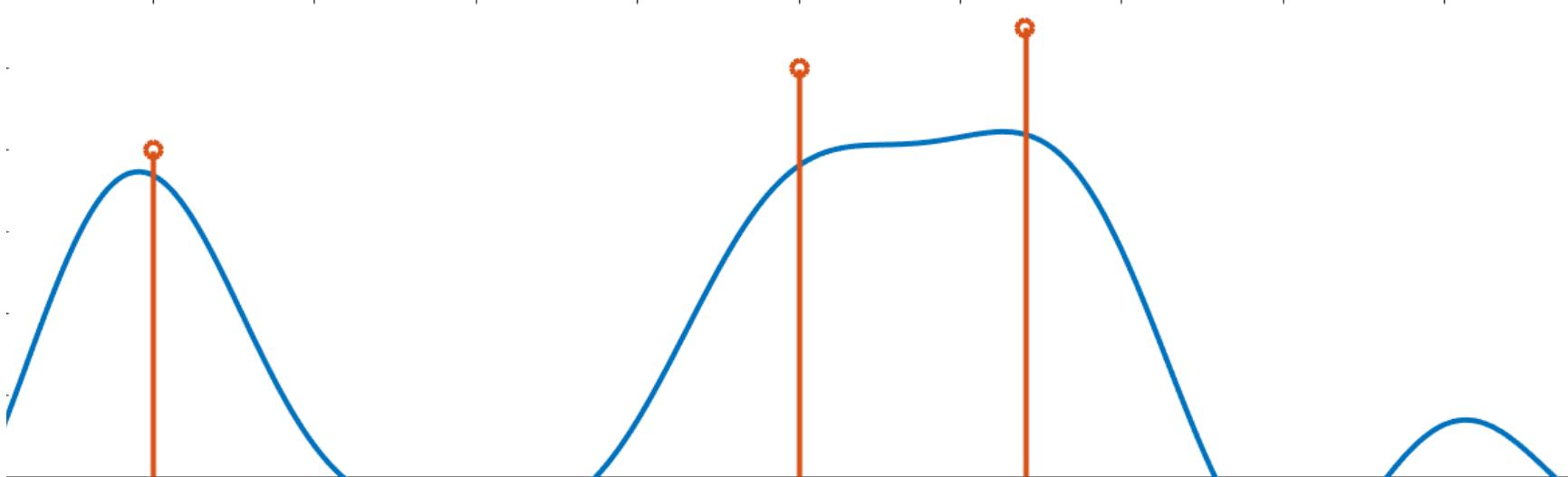
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Discretise on a fine grid?

Approach: Discrete Φ on a fine grid

For $\phi(x) \in \mathbb{R}^m$, define: $A = [\phi(x_1), \phi(x_2), \dots, \phi(x_N)] \in \mathbb{R}^{m \times N}$

$$\min_{x \in \mathbb{R}^n} F(x) = \frac{1}{2\lambda} \|Ax - y\|^2 + \|x\|_1$$



Example: Fourier measurements

$$\text{Column } i : A_i = \left(\exp(2\pi\sqrt{-1}x_i^\top \omega_k) \right)_k$$

$\mathcal{O}(p^{-d})$ grid points if $[x_i] \subseteq [0,1]^d$ spaced p apart

Forward-Backward splitting

$$\min_x F(x) := f(x) + g(x)$$

Assume that f is differentiable

Forward-Backward splitting:

$$\begin{cases} \hat{x}_{k+1} &= x_k - \tau \nabla f(x_k) \\ x_{k+1} &= \text{Prox}_{\tau g}(\hat{x}_{k+1}) := \operatorname{argmin}_z \frac{1}{2\tau} \|z - \hat{x}_{k+1}\|^2 + g(z) \end{cases}$$

Assume:

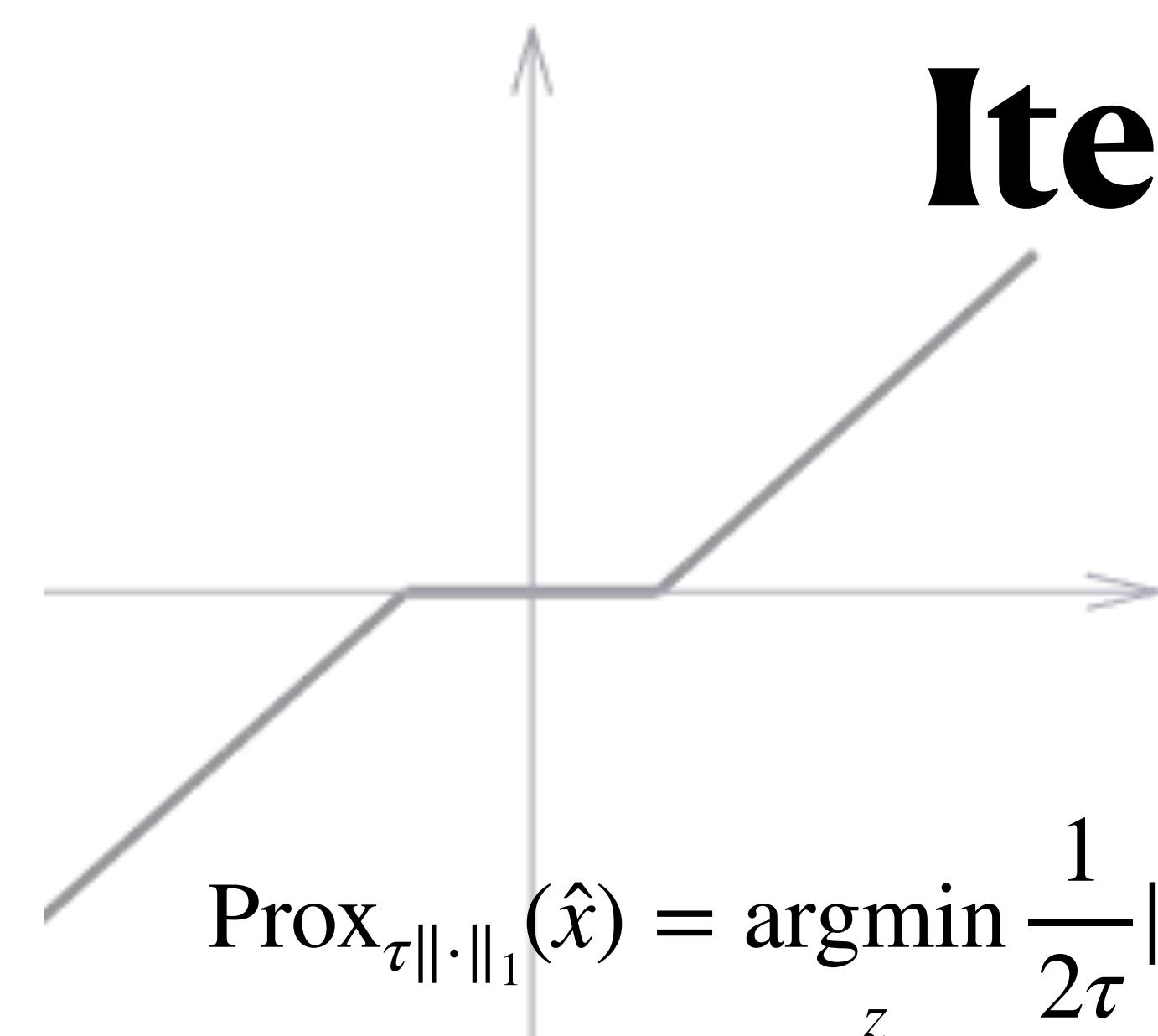
- f, g convex
- $\|\nabla f(x) - \nabla f(x')\| \leq L\|x - x'\|$



Convergence rates: If $\tau = 1/L$, then

$$F(x_k) - \min_x F(x) \leq \frac{L}{k}$$

Iterative Soft Thresholding



$$\begin{aligned}\text{Prox}_{\tau \|\cdot\|_1}(\hat{x}) &= \operatorname{argmin}_z \frac{1}{2\tau} \|z - \hat{x}\|^2 + \|z\|_1 \\ &= \text{sign}(\hat{x})(|\hat{x}| - \tau)_+\end{aligned}$$

$$\begin{cases} \hat{x}_{k+1} &= x_k - \tau A^\top (Ax_k - y) \\ x_{k+1} &= \text{Prox}_{\tau \|\cdot\|_1}(\hat{x}_{k+1}) \end{cases}$$

$$f(x) = \frac{1}{2} \|Ax - y\|^2 \text{ is } L\text{-Lipschitz with } L = \|A\|^2$$

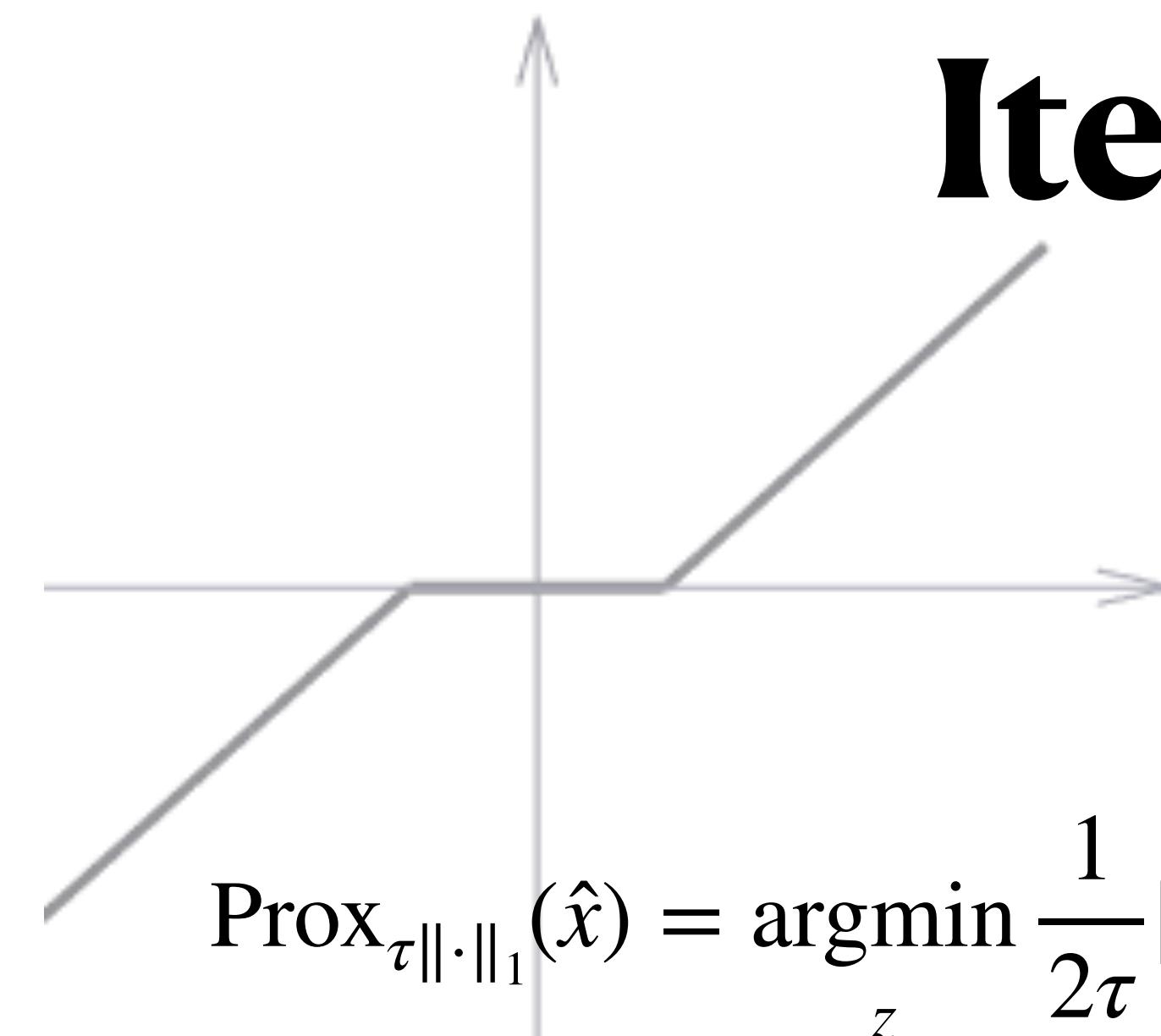
Convergence rates: for $\tau = 1/L$

$$F(x_k) - \min_x F(x) \leq \frac{\|A\|^2}{k}$$

Example: Fourier measurements

$$\begin{aligned}\text{Column i : } A_i &= \left(\exp(2\pi\sqrt{-1}x_i^\top \omega_k) \right)_k \\ \|A\|^2 &= \mathcal{O}(p^{-d})\end{aligned}$$

Iterative Soft Thresholding



$$\min_{x \in \mathbb{R}^n} \Phi(x) = \frac{1}{2\lambda} \|Ax - y\|^2 + \|x\|_1$$

$$\begin{aligned}\text{Prox}_{\tau\|\cdot\|_1}(\hat{x}) &= \operatorname{argmin}_z \frac{1}{2\tau} \|z - \hat{x}\|^2 + \|z\|_1 \\ &= \operatorname{sign}(\hat{x})(|\hat{x}| - \tau)_+\end{aligned}$$

$$\begin{cases} \hat{x}_{k+1} &= x_k - \tau A^\top (Ax_k - y) \\ x_{k+1} &= \text{Prox}_{\tau\|\cdot\|_1}(\hat{x}_{k+1}) \end{cases}$$

Convergence rates (depends on n):

$$F(x_k) - \min_x F(x) \leq \frac{C_n}{k}$$

NB: C_n can grow with n !

Grid-free convergence rates (Chizat 2021):

$$F(x_k) - \min_x F(x) \leq k^{-2/(d+1)}$$

NB: Result is independent of n

Finite dimensional formulations

$$\sup_{p \in \mathbb{R}^m} \langle p, y \rangle - \frac{\lambda}{2} \|p\|^2 \quad \text{s.t.} \quad \|\Phi^* p\|_\infty \leq 1$$

In general, the constraint is infinite dimensional. However, there are special cases for which one can formulate as a finite dimensional problem.

Fourier setting

[Candés & Fernandez-Granda 2014]:

Minimise over all p such that for all x ,

$$\left| \sum_{|k| \leq f_c} p_k \exp(2\pi\sqrt{-1}kx) \right| \leq 1$$

This constraint can be written as a positive semidefinite constraint on matrices.

Quadratic: $\phi(x) = ((u_i^\top x)^2)_i$ for $x \in \mathbb{S}_{n-1}$, then

$$\Phi^* p(x) = \sum_k p_k (u_k^\top x)^2 = \left\langle \left(\sum_k p_k u_k u_k^\top \right) x, x \right\rangle$$

Constraint: Spectral norm is bounded by 1.

ReLU [Pilancı & Ergen 2020]: $\phi(x) = ((u_i^\top x)_+)_i$ for $x \in \mathbb{S}_{n-1}$. Then. $\Phi^* p(x) = \sum_k p_k (u_k^\top x)_+$

Uses the fact that there are only finitely many support patterns for which $(Ux)_+ \neq 0$.

Semi-definite programming

Special case of Fourier samples:

$$\text{minimise over all } p \text{ such that for all } x, \quad \left| \sum_{|k| \leq f_c} p_k \exp(2\pi\sqrt{-1}kx) \right| \leq 1$$

Theorem (Dumitrescu): A trigonometric polynomial $f(t) = \sum_{k=0}^{n-1} c_k \exp(\sqrt{-1}2\pi kx)$ with $p \in \mathbb{C}^n$ is uniformly bounded by 1 in magnitude if there exists $Q \in \mathbb{C}^{n \times n}$ Hermitian s.t.

$$0 \preceq \begin{pmatrix} Q & p \\ p^* & 1 \end{pmatrix} \quad \text{and} \quad \sum_{i=1}^{n-j} Q_{i,i+j} = \delta_{0,j}$$

Semi-definite programming

Equivalent dual formulation: Let $n = 2f_c + 1$:

$$\sup_{p,Q} \langle p, y \rangle - \frac{\lambda}{2} \|p\|^2 \quad \text{s.t.} \quad 0 \leq \begin{pmatrix} Q & p \\ p^* & 1 \end{pmatrix} \quad \text{and} \quad \sum_{i=1}^{n-j} Q_{i,i+j} = \delta_{0,j}$$

Finite dimensional semi-definite program!

1. Solve SDP to find p_λ
2. Find the support of m_λ by finding the roots of the polynomial
$$F_{2n-2}(e^{\sqrt{-1}2\pi x}) = 1 - |\Phi^* p_\lambda(x)|^2$$
3. This has at most $n - 1$ roots (unless identically 0)
4. Solve for amplitudes.

Frank-Wolfe algorithm

$$\min_{x \in C} f(x)$$

C is a weakly compact convex set of a Banach space.
 f is a differentiable convex function.

1. $z^k \in \operatorname{argmin}_{z \in C} f(x^k) + \langle \nabla f(x^k), z - x^k \rangle$
2. If $\langle \nabla f(x^k), z^k - x^k \rangle = 0$ then x^k is a solution.
3. $\gamma^k = 2/(k + 2)$
4. $x^{k+1} = x^k + \gamma^k(z^k - x^k)$

- f is convex $\implies f(z) \geq f(x^k) + \langle \nabla f(x^k), z - x^k \rangle \stackrel{\text{Step 2}}{\implies} f(z) \geq f(x^k)$ for all z .
- One can replace x^{k+1} in step 4 with any \hat{x}^{k+1} such that $f(\hat{x}^{k+1}) \leq f(x^{k+1})$.

Applying Frank-Wolfe to the Blasso

$$\mu \in \operatorname{argmin}_{\mu \in \mathcal{M}(\mathcal{X})} f_\lambda(m) := \frac{1}{2} \|\Phi\mu - y\|^2 + \lambda \|\mu\|_{TV}$$

$$(\|\mu\|_{TV}, \mu) \in \operatorname{argmin}_{(t, \mu) \in C} \hat{f}_\lambda(t, \mu) := \frac{1}{2} \|\Phi\mu - y\|^2 + \lambda t$$

$$C = \{(t, \mu) \in \mathbb{R}_+ \times \mathcal{M}(\mathcal{X}) : \|\mu\|_{TV} \leq t \leq \|y\|^2/(2\lambda) =: M\}$$

\hat{f}_λ is differentiable :

$$\begin{cases} \partial_t \hat{f}_\lambda = \lambda \\ \partial_\mu \hat{f}_\lambda(t, \mu) = \Phi^*(\Phi\mu - y) \end{cases}$$

$\mu \in \operatorname{argmin} f_\lambda(\mu)$ implies

$$\begin{aligned} \lambda \|\mu\|_{TV} &\leq \lambda \|\mu\|_{TV} + \frac{1}{2} \|\Phi\mu - y\|^2 \\ &\leq \lambda \|0\|_{TV} + \frac{1}{2} \|\Phi 0 - y\|^2 = \frac{1}{2} \|y\|^2 \end{aligned}$$

Convergence of Frank-Wolfe

[Jaggi (2011)]: The curvature constant of f over C is

$$R := \max_{\substack{\gamma \in [0,1] \\ x, s, y \in C}} \frac{2}{\gamma^2} (f(y) - f(x) - \langle \nabla f(x), y - x \rangle)$$
$$y = (1 - \gamma)x + \gamma s$$

Convergence rate:

$$f(x^k) - f^* \leq \frac{2R}{k+2}$$

- $R = 0$ if f is linear
- ∇f is L -Lipschitz $\implies f(y) - f(x) - \langle \nabla f(x), y - x \rangle \leq \frac{L}{2} \|y - x\|^2$ $\implies R \leq L \text{diam}(C)^2$
- For \hat{f}_λ , $R = \frac{1}{2} \sup \{ \|\Phi(m - m')\|^2 : \|m\|_{TV}, \|m'\|_{TV} \leq \|y\|^2/2 \}$
- If $\|\phi(x)\| = 1$ for all x , then $R \lesssim \|y\|^2$ and the convergence rate is $\mathcal{O}(\|y\|^2/k)$

Applying Frank-Wolfe to the Blasso

Key step.

Let $u^k = (t^k, m^k)$.

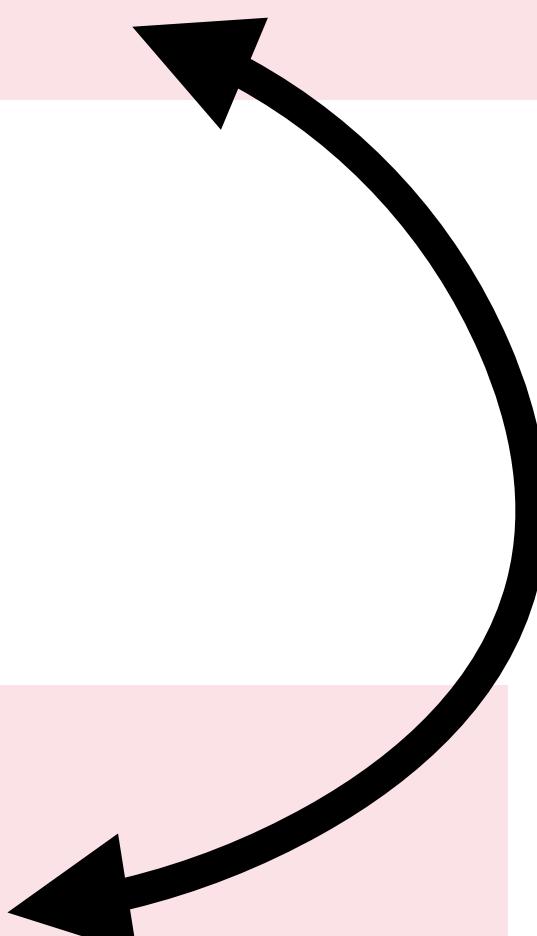
$$z^k \in \operatorname{argmin}_{z \in C} \hat{f}(u^k) + \langle \nabla \hat{f}(u^k), z - u^k \rangle$$

$$= \operatorname{argmin}_{(t,m) \in C} \langle \Phi^*(\Phi m^k - y), m \rangle + \langle \lambda, t \rangle$$

$$x^k \in \operatorname{argmin}_{x \in \mathcal{X}} \pm [\Phi^*(\Phi m^k - y)](x) + \lambda$$

$$= \operatorname{argmax}_{x \in \mathcal{X}} |\eta^k(x)|, \quad \eta^k = \frac{1}{\lambda} [\Phi^*(\Phi m^k - y)]$$

$$a^k = -\operatorname{sign}(\eta^k(x^k)) M$$



C is a convex set and minimum is achieved at an extremal point of C .

$$E = \{(M, \pm M\delta_x) : x \in \mathcal{X}\}$$

$$\implies z^k = (M, \pm M\delta_{x_k})$$

Applying Frank-Wolfe to the Blasso

At each iteration k , $\mu^{k-1} = \sum_{j=1}^{k-1} a^j \delta_{x^j}$

Define $\eta^k = \frac{1}{\lambda} [\Phi^*(\Phi\mu^{k-1} - y)]$ and $\gamma^k = 2/(k+2)$.

1. Add new spike: $x^k = \operatorname{argmax}_{x \in \mathcal{X}} |\eta^k(x)|$

2. $\mu^k = \mu^{k-1} + \gamma^k (a_k \delta_{x^k} - \mu^{k-1})$

Terminate if $\eta^k(x^k) = \pm 1$ and return μ^k

Sliding Frank-Wolfe: [Denoyelle et al 2018]

Replace step 2 with any $\hat{\mu}^k$ such that $f_\lambda(\hat{\mu}^k) \leq f_\lambda(\mu^k)$:

$$\hat{\mu}^k = \sum_{j=1}^k \hat{a}_j \delta_{\hat{x}_j} \text{ where}$$

$$(\hat{a}, \hat{x}) \in \min_{a, x} \lambda \|a\|_1 + \frac{1}{2} \|\Phi \mu_{a,x} - y\|^2$$

Theorem (Denoyelle et al, 2019): finite convergence if η_V is non-degenerate at the solution.

Remarks

- The sliding Frank-Wolfe is an off-the-grid algorithm, however:
 - the **difficulty** is in the step $x^k = \operatorname{argmax}_{x \in \mathcal{X}} |\eta^k(x)|$
- \mathcal{X} is a continuous space and η^k is a continuous (smooth) function
- In practice, discretize \mathcal{X} and do a local ascent step on η^k
- This is computationally intensive if $\mathcal{X} \subset \mathbb{R}^d$ and d is large.

Particle methods

$$\min_{\mu} \lambda \|\mu\|_{TV} + \frac{1}{2} \|\Phi\mu - y\|^2$$

This has a solution consisting of $m + 1$ Diracs

$$\min_{a,x} \lambda \sum_{i=1}^k |a_i| + \frac{1}{2} \left\| \sum_{i=1}^k \phi(x_i) a_i - y \right\|^2$$

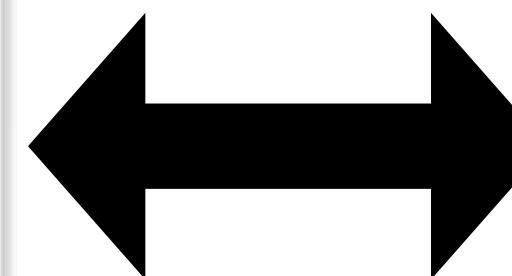
Has the same value as $P_\lambda(y)$ when $k \geq m$

Chizat and Bach (2018): Global convergence results for *sufficiently large k* .

VarPro

[Golub and Pereyra, 1978]

$$\min_{a,x} \left\| \sum_{j=1}^K \phi(x_j) a_j - y \right\|^2$$



$$\begin{aligned} & \min_x f(x) \text{ where} \\ & f(x) = \min_a \left\| \sum_j \phi(x_j) a_j - y \right\|^2 \end{aligned}$$

Easy to compute gradient:

$$\partial_{x_j} f(x) = \partial_{x_j} \left\| \Phi_x \bar{a} - y \right\|^2 = \bar{a}_j \nabla \phi(x_j)^\top (\Phi_x \bar{a} - y)$$

$$\bar{a} = \operatorname{argmin}_a \left\| \Phi_x a - y \right\|^2 = \Phi_x^\dagger y$$

In general, solution is non-sparse.

Leads to better problem conditioning.

VarPro

A practical approach for **sparse solutions** (Nonsmooth VarPro):

$$\min_x f(x) \text{ where } f(x) := \min_a \frac{1}{2} \|\Phi_x a - y\|^2 + \lambda \|a\|_1$$

If the inner Lasso problem has a unique solution for x , then f is differentiable at x with gradient

$$\partial_{x_j} f(x) = \partial_{x_j} \|\Phi_x \bar{a} - y\|^2 = \bar{a}_j \nabla \phi(x_j)^\top (\Phi_x \bar{a} - y)$$

$$\bar{a} = \operatorname{argmin}_a \frac{1}{2} \|\Phi_x a - y\|^2 + \lambda \|a\|_1$$

Summary

- For certain settings (Fourier sampling), one can convert to a finite dimensional optimisation problem.
- The Frank-Wolfe algorithm is a versatile algorithm for computations off-the-grid. Works well in low dimensions, but there is a difficulty with finding the argmax of η_k
- Particle methods are effective in practice, but no quantitative rates.

References

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