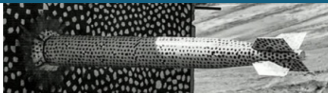
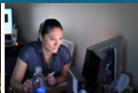




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Using Filter Methods to Guide Convergence for ADMM, with Applications to Nonnegative Matrix Factorization Problems



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ICCOPT 2022 - Nonlinear Optimization

Bethlehem, PA



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Introduction

Background

Augmented Lagrangians
Filters

Algorithm

Bilinear NMF/C Example

Spectra

Conclusions

- ▶ Nonlinear Programs (NLP):

$$\begin{array}{ll} \text{minimize}_{\mathbf{x}} & f(\mathbf{x}) \\ \text{such that} & c(\mathbf{x}) = 0 \\ & \mathbf{x} \in \mathcal{X} \end{array} \quad (1)$$

- ▶ $\mathbf{x} := [x_0; \dots; x_p] \in \mathbb{R}^n$ for p blocks ($n = \sum_{i=0}^p n_i$), $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $c : \mathbb{R}^n \rightarrow \mathbb{R}^m$, $\mathcal{X}$ simple bounds.
- ▶ We assume $f, c \in \mathcal{C}^2$; f, c possibly separable.

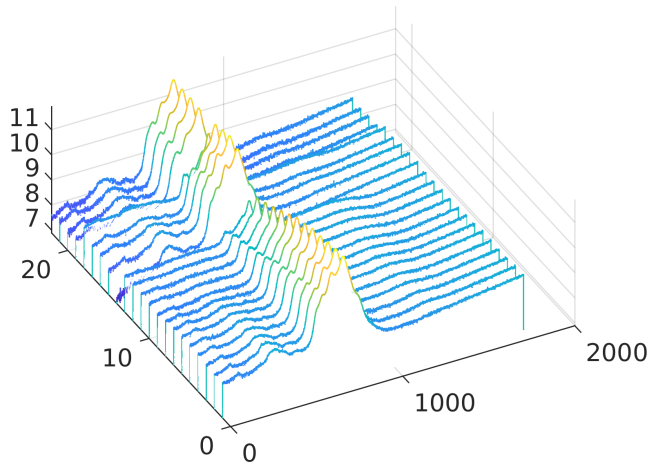
Motivating Example - Chemical Spectrum Analysis



- ▶ Find distributions of chemicals that occur in measured spectrum analysis.
- ▶ Each chemical follows a Gaussian distribution; need nonnegative combination of Gaussians that reproduce the spectra data.
- ▶ *Intensity Function* as a function of wave number w and concentration c , with rank constraint K . For m be the number of concentrations c :

$$\hat{l}(w_i, c_j) = \sum_{k=1}^K \underbrace{Y_{k,j}}_{f_k(c_j)} \underbrace{\exp\left(-\frac{1}{2} \left(\frac{w_i - \mu_k}{\sigma_k}\right)^2\right)}_{g_k(w_i)} \quad (2)$$

- ▶ Built “image” from mean, standard deviations, and nonnegative coefficients



Spectra data: $M \in \mathbb{R}^{1750 \times 22}$, concentration (x-axis) $\times$ wavelength (y-axis) $\times \hat{I}(z)$.

- ▶ First utilized in Douglas and Rachford [1956], extended as method for variational problems in Gabay and Mercier [1975], Glowinski and Marroco [1975].
- ▶ Classical ADMM takes the form of a 2-block update

$$\min_{\mathbf{x} := [x_1, x_2]} f(\mathbf{x}) := f_1(x_1) + f_2(x_2) \quad \text{subject to} \quad c(\mathbf{x}) := A_1 x_1 + A_2 x_2 - b = 0. \quad (3)$$

- ▶ Most literature assumes $c(\mathbf{x}) = \mathbf{Ax} - b$ or linear constraints, and $f = f_1 + f_2$.

7 Direct multiblock extension



- ▶ Now $\mathbf{x} = [x_1, \dots, x_p]$,

$$\min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}) \quad \text{s.t.} \quad A_0 x_0 + \dots + A_p x_p = \mathbf{b}. \quad (4)$$

simple constraint sets $\mathcal{X}$ (e.g., bounds), multiaffine $c(\mathbf{x})$ as in Gao et al. [2020].

- ▶ Block-minimize the augmented Lagrangian for (4)

$$\mathcal{L}_\rho(\mathbf{x}, \mathbf{y}) = f(\mathbf{x}) + \mathbf{y}^T (\mathbf{A}\mathbf{x} - \mathbf{b}) + \frac{\rho}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 \quad (5)$$

- ▶ The classical 2-block problem differs greatly; Chen et al. [2016] provides example $p = 3$ blocks $f_1, f_2, f_3 \equiv 0$ where ADMM diverges for any ρ .
- ▶ Nonconvex settings Wang et al. [2018]: NMF/C, phase retrieval, consensus problems.

Algorithm 1: Basic ADMM P-Block splitting for (4)

Data: functions f , matrices $\mathbf{A}$, vector $\mathbf{b}$, augmented Lagrangian parameter $\rho > 0$, and initial $\mathbf{x}_0, y_0$

Result: $\mathbf{x} \leftarrow \arg \min_{\mathbf{x}} f(\mathbf{x})$ s.t. $\mathbf{Ax} = \mathbf{b}$ in (4)

for $k = 0, 1, \dots$ **do**

for $i = 1, \dots, p$ **do**

$\mathbf{x}_i^{(k+1)} = \arg \min_{\mathbf{x}_i} \mathcal{L}_\rho([\mathbf{x}_{<i}^{(k)}, \mathbf{x}_i^{(k)}, \mathbf{x}_{>i}^{(k)}], y^{(k)})$

end

$y^{(k+1)} = y^{(k)} + \rho(\mathbf{Ax}^{(k+1)} - \mathbf{b})$

end



- ▶ Literature: ADMM convergence is still “somewhat” nebulous: requires *a priori* knowledge of functions, ρ choice is largely open, limited choices in $c(\mathbf{x})$.
- ▶ Tools:
 - ▶ Augmented Lagrangian, ADMM/block-updates, Filter Methods

Problem: can we solve nonconvex, nonlinear problems (1) with block structure?

- ▶ What about nonconvex/nonlinear constraints?
- ▶ Can filters help guide convergence?



- ▶ Lagrangian of NLP (1)

$$\mathcal{L}(\mathbf{x}, y) = f(\mathbf{x}) + y^T c(\mathbf{x}) \quad (6)$$

where $y \in \mathbb{R}^m$ is the vector of Lagrange multipliers of $c(\mathbf{x})$.

- ▶ $\mathcal{X} \subseteq \mathbb{R}^n$ is a simple feasible set:

$$\text{proj}_{\mathcal{X}}(\mathbf{x}) \equiv \arg \min_{y \in \mathcal{X}} \|\mathbf{y} - \mathbf{x}\| \quad (7)$$

- ▶ First-order optimality & feasibility (w/ $\mathcal{X}$ simple bounds $l \leq \mathbf{x} \leq u$):

$$\text{proj}_{\mathcal{X}}(\mathbf{x} - \nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, y)) - \mathbf{x} = 0 \quad \Rightarrow \quad \min\{\mathbf{x} - l, \max\{\mathbf{x} - u, \nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, y)\}\} = 0 \quad (8a)$$

$$c(\mathbf{x}) = 0 \quad (8b)$$

Augmented Lagrangian Methods



- Adds quadratic penalty term to (6):

$$\mathcal{L}_\rho(\mathbf{x}, y) = \underbrace{f(\mathbf{x}) - y^T c(\mathbf{x})}_{\mathcal{L}_0(\mathbf{x}, y)} + \frac{1}{2}\rho \|c(\mathbf{x})\|^2 \quad (9)$$

for a penalty parameter ρ .

- Bound Constrained Aug-Lag:

$$\min_{\mathbf{x}} \quad \mathcal{L}_{\rho_k}(\mathbf{x}, y^{(k)}) \quad (10a)$$

$$\text{such that} \quad l \leq \mathbf{x} \leq u \quad (10b)$$

for fixed ρ_k and $y^{(k)}$.

- Solve (10), and then

$$y^{(k+1)} = y^{(k)} - \rho c(\mathbf{x}^{(k+1)})$$

- $y^{(k)}$ update makes dual feasible, primal feasibility in limit



- ▶ Backbone for solving nonlinear problems Vanaret and Leyffer [2020]:
 - ▶ Interior-point methods; most used for large-scale problems
 - ▶ Active-set methods; great for warm-starts
 - ▶ Issues: lack warm-starts (IP) and cannot scale (AS)

Goal: Leverage different solver flexibilities for nonlinearities in f and c

- ▶ *But*: need scaling capabilities for independent block updates - destroyed by quadratic term

Filter Methods



- ▶ Monitoring trade-off between primal feasibility and first-order convergence.
- ▶ η and ω represent infeasibility and first order error:

$$\eta(\mathbf{x}) := \|\mathbf{c}(\mathbf{x})\| \quad (11a)$$

$$\omega(\mathbf{x}, \mathbf{y}) := \left\| \underset{\mathcal{X}}{\text{proj}}(\mathbf{x} - \nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \mathbf{y})) - \mathbf{x} \right\| \quad (11b)$$

- ▶ Keep track of (ω_0, η) pairs, update $\mathbf{y}^{(k)}$ when reach acceptable point or ρ_k if not feasible enough

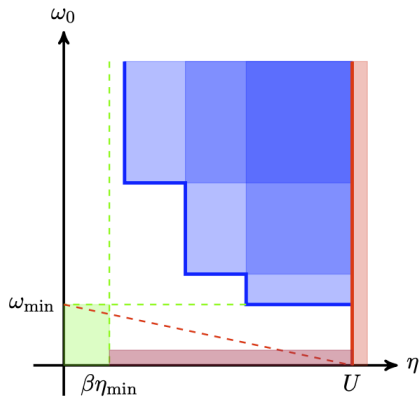
Definition (Augmented Lagrangian Filter and Acceptance)

A filter $\mathcal{F}$ is a list of pairs $(\eta_l, \omega_l) := (\eta(\mathbf{x}^{(l)}), \omega_0(\mathbf{x}^{(l)}, \mathbf{y}^{(l)}))$ such that no pair dominates another pair, i.e., there exists no pairs $(\eta_l, \omega_l), (\eta_k, \omega_k)$, $l \neq k$ such that $\eta_l \leq \eta_k$ and $\omega_l \leq \omega_k$. A point $(\mathbf{x}^{(k)}, \mathbf{y}^{(k)})$ is acceptable to the filter $\mathcal{F}$ iff

$$\eta_k := \eta(\mathbf{x}^{(k)}) \leq \beta \eta_l \text{ or } \omega_k := \omega_0(\mathbf{x}^{(k)}, \mathbf{y}^{(k)}) \leq \omega_l - \gamma \eta(\mathbf{x}^{(k)}) \quad (12)$$

$\forall (\eta_l, \omega_l) \in \mathcal{F}$ where $0 < \gamma, \beta < 1$.

Filter Example



(a) Filter is blue; U is upper bound ($\eta(\mathbf{x}) \leq U := \max(\omega_{\min}/\gamma, \beta\eta_{\min})$). Values in the blue are not acceptable; shaded purple triggers restoration.



- ▶ Monitors dual infeasibility error of the original problem while solving the augmented Lagrangian.
- ▶ Restoration conditions

$$\eta(\mathbf{x}) = \eta(\mathbf{x}^{(j+1)}) \geq \beta U \quad (13a)$$

$$\omega_{\rho_k}(\mathbf{x}^{(j+1)}, y^{(k)}) \leq \epsilon \quad \text{and} \quad \eta(\mathbf{x}^{(j+1)}) \geq \beta \eta_{\min}. \quad (13b)$$

- ▶ *Optimal* stopping criteria: relative first order error ω_{ρ_k} (11b)

$$\frac{\|\text{proj}_{\mathcal{X}}(\mathbf{x} - \nabla_{\mathbf{x}} \mathcal{L}_0(\mathbf{x}^{(k)}, y^{(k)})) - \mathbf{x}\|}{\|\text{proj}_{\mathcal{X}}(\mathbf{x} - \nabla_{\mathbf{x}} \mathcal{L}_0(\mathbf{x}^{(0)}, y^{(0)})) - \mathbf{x}\|} = \frac{\omega_0(\mathbf{x}_k, y_k)}{\omega_0(\mathbf{x}_0, y_0)} \leq \varepsilon \quad (14)$$

where $\mathbf{x}^{(0)}$ is the initial iterate.

Algorithm 2: Outline of ADMM-F for (1)

```
while  $(x^{(k)}, y^{(k)})$  not optimal (14) do
  while  $(\eta^{(j)}, \omega^{(j)})$  not acceptable to  $\mathcal{F}_k$  do
    while ! Satisfied do
      for  $i = 1, \dots, p$  with  $p$  blocks do
        if  $j == 0$  then
           $x_i^{(j+1)} \leftarrow \text{proj}_{\mathcal{X}_i}(x_i^{(j)} - \alpha_i \nabla_i \mathcal{L}_{\rho_k}([x_{<i}^{(j+1)}, x_i^{(j)}, x_{>i}^{(j)}], y^{(k)}))$  // Block coordinate steepest descent
        else
           $x_i^{(j+1)} \leftarrow \arg \min_{x_i \in \mathcal{X}_i} \mathcal{L}_{\rho_k}([x_{<i}^{(j+1)}, x_i, x_{>i}^{(j)}], y^{(k)})$ 
        end
      end
      end
      if Restoration condition (13) holds then
        Find  $x^{(j+1)}$  s.t.  $(\eta^{(j+1)}, \omega^{(j+1)}) \in \mathcal{F}_k$ , or  $x^{(j+1)} \leftarrow \arg \min_{x \in \mathcal{X}} \|c(x)\|^2$ ;
        // exits Filter/j-loop
      else
        Compute  $\omega_{\rho_k}(x^{(j)}, y^{(k)}), \eta(x^{(j)}, y^{(k)})$ ;
      end
    end
    if  $\eta^{(k)} > 0$  then
      Add  $(\eta^{(k)}, \omega^{(k)})$  to  $\mathcal{F}_k$ 
      Update:  $(\eta^{(k)}, \omega^{(k)}) \leftarrow (\omega_{\rho_k}(x^{(k+1)}, y^{(k+1)}), \eta(x^{(k+1)}, y^{(k+1)}))$ ;
    end
    if Entered Restoration then
      Increase Penalty  $\rho_{k+1} \leftarrow \max(\rho_k, \xi \rho_k)$ ;
    end
  end
end
```

Assumption (Differentiability & Set compactness)

Consider (1), and assume that f and c are continuously differentiable. In addition, the constraint norm satisfies $\|c(\mathbf{x})\| \rightarrow \infty$ as $\|\mathbf{x}\| \rightarrow \infty$.

Assumption 1 implies that our iterates remain in a compact set, replaced with finite bounds $l \leq \mathbf{x} \leq u$. Assumption 1 implies that f , c , and their derivatives are bounded for all iterates. Algorithm 2 has three distinct outcomes:

1. There exists an infinite sequence of restoration phase iterates $\mathbf{x}^{k_l}$, indexed by $\mathcal{R} := \{k_1, k_2, \dots\}$, whose limit point $\mathbf{x}^* := \lim \mathbf{x}^{k_l}$ minimizes the constraint violation, satisfying $\eta(\mathbf{x}^*) > 0$.
2. There exists an infinite sequence of successful major iterates $\mathbf{x}^{k_l}$, indexed by $\mathcal{S} := \{k_1, k_2, \dots\}$, and the linear independence constraint qualification (LICQ) fails to hold at the limit $\mathbf{x}^* := \lim \mathbf{x}^{k_l}$, which is a Fritz-John (FJ) point of (1).
3. There exists an infinite sequence of successful major iterates $\mathbf{x}^{k_l}$, indexed by $\mathcal{S} := \{k_1, k_2, \dots\}$ and LICQ holds at the limit $\mathbf{x}^* := \lim \mathbf{x}^{k_l}$, which is a KKT point of (1).



Theorem

Under Assumption 1, either Algorithm 2 terminates after a finite number of iterations at a KKT point: for some k , $\mathbf{x}^{(k)}$ is a first-order stationary point with $\eta(\mathbf{x}^{(k)}) = 0$ and $\omega(\mathbf{x}^{(k)}) = 0$, or there exists an infinite sequence of iterates $\mathbf{x}^{(k)}$ and any limit point $\mathbf{x}^{(k)} \rightarrow \mathbf{x}^$ that satisfy one of the following:*

- 1. The penalty parameter is updated finitely often, and $\mathbf{x}^*$ is a KKT point;*
- 2. There exists an infinite sequence of restoration steps at which the penalty parameter is updated. If $\mathbf{x}^*$ satisfies the LICQ, it is a KKT point; otherwise, it is an FJ point;*
- 3. The restoration phase converges to a minimum of the constraint violation.*

- We establish a generalized Cauchy point with projected gradient descent Beck and Tetruashvili [2013, Lemma 3.3].

$$\mathbf{x}_i^{(j+1)} \leftarrow \text{proj}_{\mathcal{X}_i} \left(\mathbf{x}_i^{(j)} - (1/L_i) \nabla_i \mathcal{L}(\mathbf{x}_i^{(j)}) \right), \quad d_i \left(\mathbf{x}_i^{(j)} \right) = \mathbf{x}_i^{(j+1)} - \mathbf{x}_i^{(j)} \quad (15)$$

Lemma

[Block Coordinate Descent Sufficient Decrease] Let $\{\mathbf{x}^{(j)}\}_{j \geq 0}$ be the sequence generated by taking one sequence of projected gradient steps (15) in each block $i = 1, \dots, p$. Then

$$\mathcal{L}(\mathbf{x}^{(j)}) - \mathcal{L}(\mathbf{x}^{(j+1)}) \geq \frac{\sigma_{\min}}{2 \left[1 + (p-1) \left(\frac{L}{L_{\min}} \right)^2 \right]} \left\| d \left(\mathbf{x}^{(j)} \right) \right\|^2. \quad (16)$$

for L the Lipschitz constant of $\mathcal{L}(\cdot)$, $L_{\min} = \min_{i \in \{1, \dots, p\}} L_i$, for L_i block Lipschitz constants, and $\sigma_{\min} = \min_{i \in \{1, \dots, p\}} \sigma_i$.



- ▶ ADMM/BCD - solves multiblock problems, parallelizable
 - ▶ Requires BCD satisfies a sufficient decrease condition.
- ▶ Filter - maintains feasibility, can handle nonlinear constraints, update ρ_k when needed
- ▶ Now - applying to bilinear NMF and extensions



- Extract from a data matrix $M \in \mathbb{R}^{N \times Q}$ two nonnegative factors $X \in \mathbb{R}^{N \times K}$, $Y \in \mathbb{R}^{K \times Q}$

$$\begin{aligned} \min_{X, Y} \frac{1}{2} \|XY - M\|_F^2 \\ \text{such that } X \geq 0, Y \geq 0 \end{aligned} \quad (17)$$

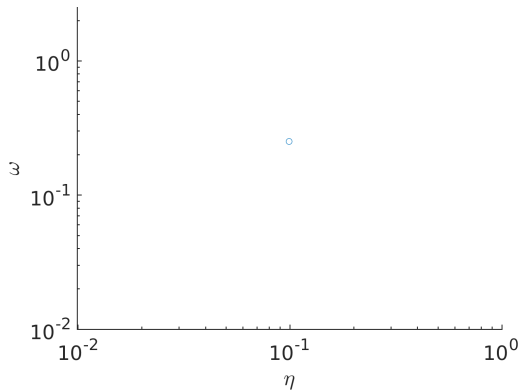
- ADMM Formulation

$$\begin{aligned} \min_{X, Y, Z} \frac{1}{2} \|Z - M\|_F^2 \\ \text{such that } X \geq 0, Y \geq 0, Z = XY \end{aligned} \quad (18)$$

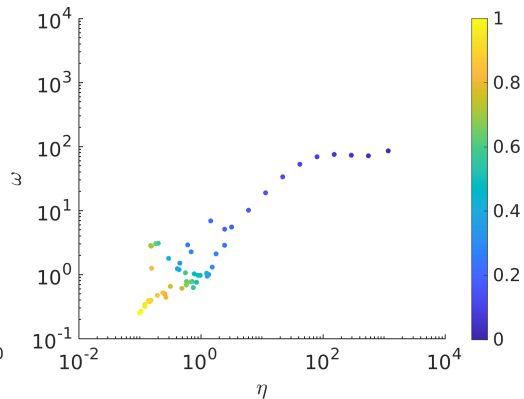
(b) *Data*(c) *XY*

NMF recapitulation of Sylvester and Filter progression through “acceptable” iterations. $M \in \mathbb{R}^{225 \times 225}$, $X \in \mathbb{R}^{225 \times 45}$. FO: $1e - 5$.

Filter Movement

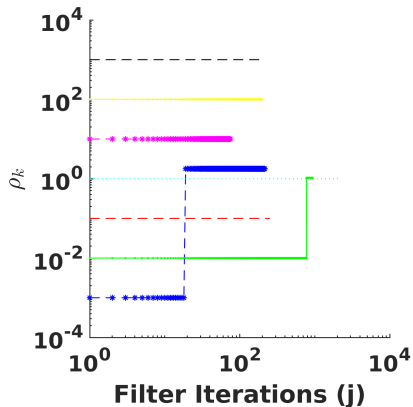
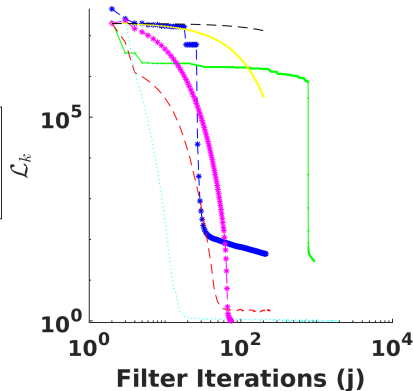
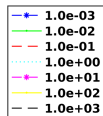
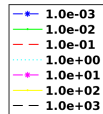


(a) Final Filter

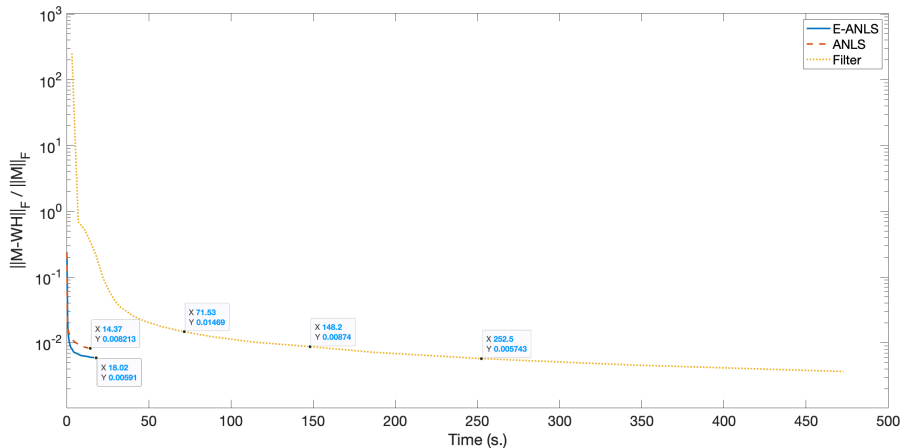


(b) Total Filter Entries with blue earliest, yellow the latest entries.

Descent and Filter Stats NMF for Sylvester T. Cat.

(a) ρ Trajectories(b) $\rho - \mathcal{L}_k$ descent

Convergence metrics for different ρ initializations.



ADMM-F Comparison with Accelerated NMF Ang and Gillis [2019]

Bilinear NMFC Problem Formulation



- ▶ Data matrix $M \in \mathbb{R}^{N \times Q}$ now contains missing values
- ▶ Need two nonnegative factors $X \in \mathbb{R}^{N \times K}$, $Y \in \mathbb{R}^{K \times Q}$ that also match observed data (via selection operator $\text{proj}_{\mathcal{X}}$)

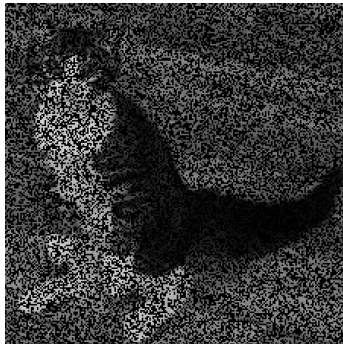
$$\min_{X, Y} \frac{1}{2} \|\text{proj}_{\mathcal{X}}(XY - M)\|_F^2, \text{ such that } X \geq 0, Y \geq 0 \quad (19)$$

- ▶ ADMM Formulation

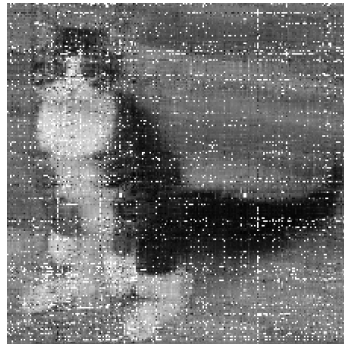
$$\begin{aligned} & \min_{X, Y, Z, W} \frac{1}{2} \|Z - W\|_F^2 \\ & \text{such that } X \geq 0, Y \geq 0 \\ & \quad Z = XY, \text{proj}_{\mathcal{X}}(W - M) = 0 \end{aligned} \quad (20)$$



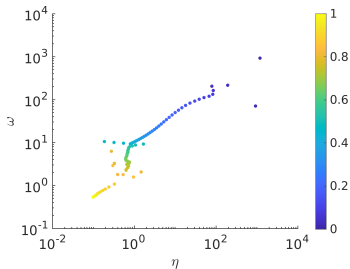
(a) True



(b) Data: 50% missing data

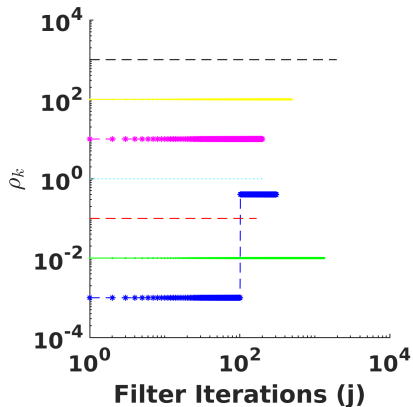


(c) XY

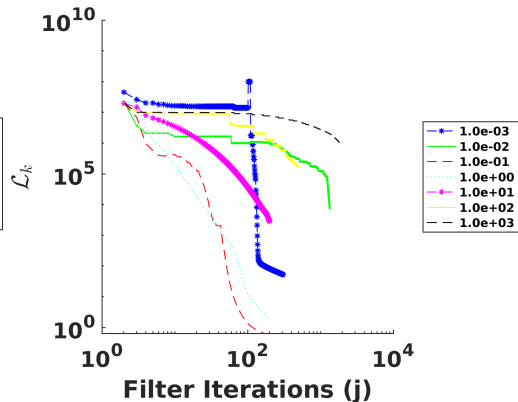


(d) Total Filter Entries: early (blue);
final (yellow)

NMFC recapitulation of Sylverster and Filter progression through “acceptable” iterations.
 $M \in \mathbb{R}^{225 \times 225}$, $X \in \mathbb{R}^{225 \times 45}$. FO: $1e - 5$.



(a) ρ Trajectories



(b) $\rho - L_k$ descent

Convergence metrics for different ρ initializations.

Chemical Spectrum - Recap

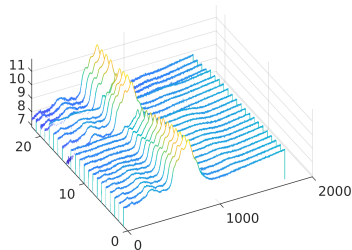


- Find distributions of chemicals that occur in measured spectrum analysis - optimize over μ, σ, Y .
- Each chemical follows a Gaussian distribution; need nonnegative combination of Gaussians that reproduce the spectra data.
- Intensity Function* as a function of wave number w and concentration c , with rank constraint K . For m be the number of concentrations c :

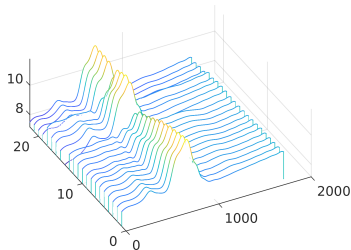
$$\hat{l}(w_i, c_j) = \sum_{k=1}^K \underbrace{h_{k,j}}_{f_k(c_j)} \underbrace{\exp\left(-\frac{1}{2} \left(\frac{w_i - \mu_k}{\sigma_k}\right)^2\right)}_{g_k(w_i)} \quad (21)$$

- Cost Function:

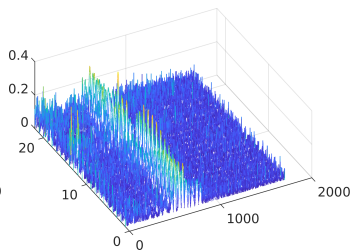
$$\min_{\mu, \sigma, Y} \sum_{i,j} (M_{i,j} - Z)^2 \quad \text{s.t.} \quad Y, \sigma \geq 0, Z = X(\mu, \sigma)Y \quad (22)$$



(a) Data

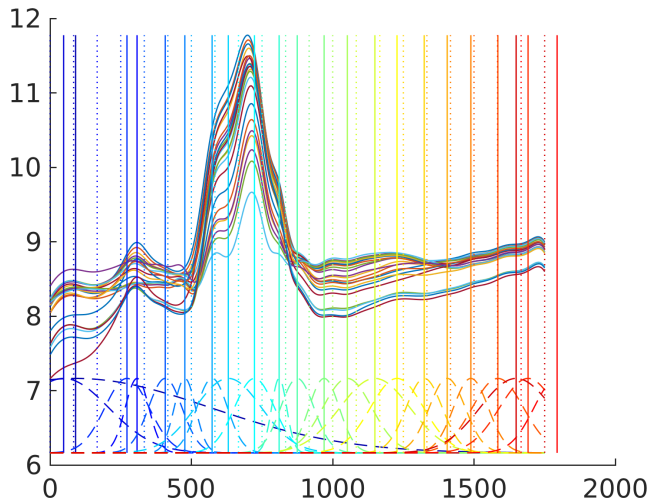


(b) XY

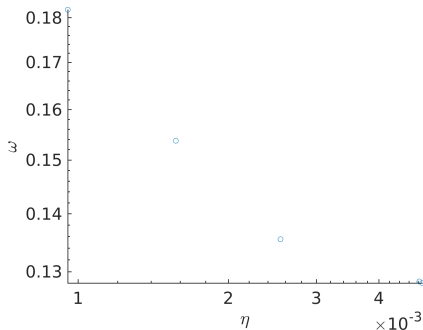


(c) Absolute Difference

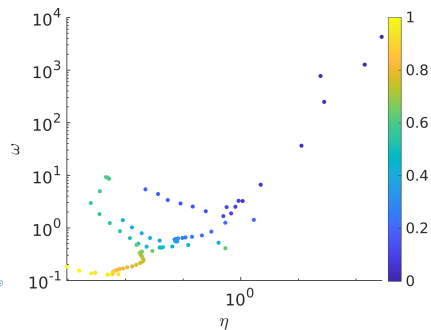
Spectra data and recapitulation through “acceptable” iterations. $M \in \mathbb{R}^{1750 \times 22}$, $X \in \mathbb{R}^{22 \times 22}$



(a) Gaussians, with mean (before ':'/after '-') and signal.

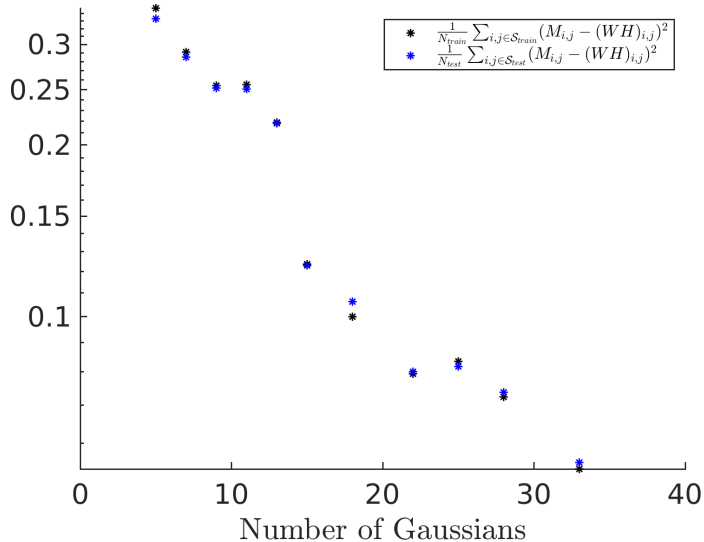


(b) Final Filter



(c) Total Filter Entries

Descent and Filter Stats for spectra inversion with 22 Gaussians.



(22) value per number of Gaussians; training & test data.



- ▶ Conclusions
 - ▶ Able to prove convergence through Filter framework
 - ▶ Filter seems able to select correct ρ values
- ▶ Theoretical - Future Directions
 - ▶ Prove Convergence w/e nonsmooth regularizers
 - ▶ BCD - already have drafted
 - ▶ Filter convergence adjustment
 - ▶ Accelerations
- ▶ Practical
 - ▶ Write real package that generalizes to nonlinear problems
 - ▶ Incorporate into existing code?

Thank you!



► Questions?



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