A Framework for Signal Decomposition with Applications to Solar Energy Generation

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Outline

What I've worked on the last 4+ years

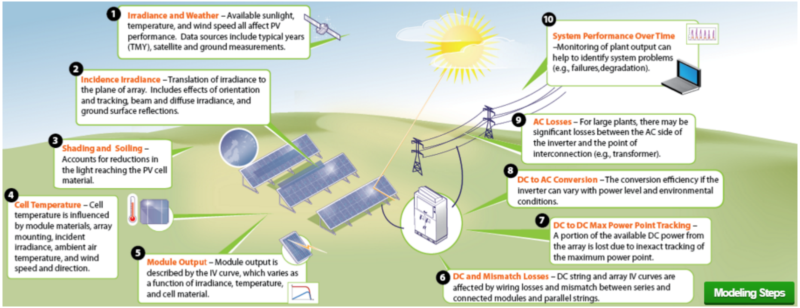
- research focused on two areas
  - optimization as a methodology for signal decomposition
  - developing useful, practical methods for solar power data science
- published 12 papers and 2 open-source software packages
- at SLAC, principle investigator on two U.S. DOE projects (SETO #34911 and #38529)

A selection of relevant papers

- B. Meyers, M. Tabone, and E. C. Kara. Statistical clear sky fitting algorithm. In *45th IEEE Photovoltaic Specialists Conference*, 2018
- B. Meyers, M. Deceglie, C. Deline, and D. Jordan. Signal processing on PV time-series data: Robust degradation analysis without physical models. *IEEE Journal of Photovoltaics*, 2019
- B. Meyers, E. Apostolaki-Iosifidou, and L. T. Schelhas. Solar data tools: Automatic solar data processing pipeline. In *47th IEEE Photovoltaic Specialists Conference*, 2020
- B. Meyers and D. J. F. Rodriguez. Estimation of shade losses in unlabeled PV data. In *49th IEEE Photovoltaic Specialists Conference*, 2022
- B. Meyers. Estimation of soiling losses in unlabeled PV data. In *49th IEEE Photovoltaics Specialists Conference*, 2022
- L. Volpatti, B. Meyers, and S. Boyd. Signal decomposition via quadratic-separable optimization. *[in progress]*, 2023
- B. Meyers and S. Boyd. Signal decomposition using masked proximal operators. *Foundations and Trends in Signal Processing*, 2023 (accepted)

- will (mostly) discuss last paper today

Motivation: Analysis of PV data



via Sandia PVPMC

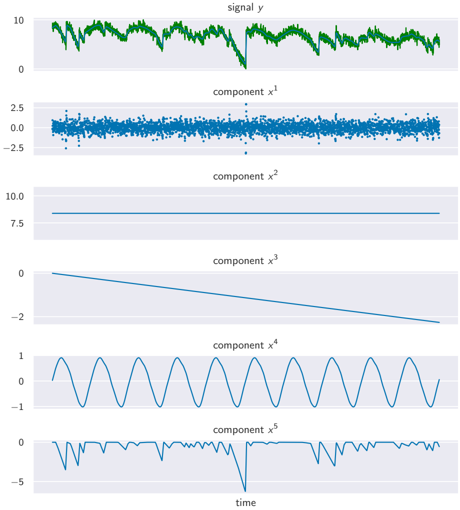
- standard approach uses photovoltaic (PV) output time series *plus*
  - location, mounting, orientation, ...
  - time series for irradiance, temperature, wind speed, ...
- can be very difficult (sometime impossible) to gather all this data
- we propose using only PV output time series, using signal decomposition

What is signal decomposition?

- given time series y
  (possibly with missing data)
- decompose as

$$y = x^1 + x^2 + \cdots + x^K$$

- components x^i have known characteristics
  - *e.g.*, smooth, periodic, nonnegative, nonincreasing, sparse, ...
- find $x^1, \ldots, x^K$ given y and characteristics
- often an underspecified problem
- raises question: how to choose one?



An age-old problem

- Babylonians use of harmonic analysis in astronomy ($\sim$1000 BCE)
- Fourier analysis in physics, astronomy (early 1800s)
- trend filtering in econometrics, earth science (1920s, formalized in 1990s)
- seasonal-trend decomposition (1920s, formalized as STL in 1990)
- sparse signal recovery in radio astronomy, JPEG standard, LASSO (1970s–1990s)
- convex demixing in geophysics (1970s)

- more recent techniques (2000–):
  - basis pursuit, dictionary learning, contextually supervised source separation, low-rank factorizations, ...

Our focus

- practical solution methods for carrying out decompositions
  - not theory and formal proofs
- specifying component characteristics via an extensible modeling language
  - not discovering components and their characteristics
- usable, open-source artifacts

```
# residual component
c1 = SumSquare(weight=1/len(y))
# constant component
c2 = NoSlope()
# linear degradation component
c3 = Aggregate([NoCurvature(), FirstValEqual(0)])
# seasonal baseline component
c4 = Aggregate([SumSquare(weight=5e0, diff=2), Periodic(365),
                AverageEqual(0, period=365)])
# soiling component
c5 = Aggregate([Inequality(vmax=0), SumAbs(weight=1e-5),
                SumQuantile(weight=1e-5, diff=1, tau=0.9),
                SumAbs(weight=5e-3, diff=2)])

problem = Problem(data=y, components=[c1, c2, c3, c4, c5])
```

Outline

Signal decomposition problem

$$\begin{array}{ll} \text{minimize} & \phi_1(x^1) + \cdots + \phi_K(x^K) \\ \text{subject to} & y_t = x_t^1 + \cdots + x_t^K, \quad t \in \mathcal{K} \end{array}$$

- data $y \in (\mathbf{R} \cup \{?\})^T$ with known entries $\mathcal{K} = \{t \mid y_t \in \mathbf{R}\}$
- variables are components $x^1, \ldots, x^K \in \mathbf{R}^T$
- components sum to signal for known entries
- component class costs $\phi_1, \ldots, \phi_K : \mathbf{R}^T \to \mathbf{R} \cup \{\infty\}$
  - $\phi_i(x)$ is the implausibility that $x^i = x$
  - infinite values encode constraints
- we choose decomposition to minimize total implausibility
- we refer to a solution as *an optimal signal decomposition*
- when class costs are convex, problem is convex

Imputing missing entries

$$y_t = x_t^1 + \cdots + x_t^K, \quad t \in \mathcal{K}$$

- decomposition gives a method for estimating missing data values, *i.e.*, *imputation*

$$\widehat{y}_t = x_t^1 + \cdots + x_t^K, \quad t \notin \mathcal{K}$$

  (recall $x^i \in \mathbf{R}^T$ have no missing values)
- provides a basis for a validation method (more on that later)

Simple class examples

mean-square small

$$\phi(x) = \frac{1}{T}\sum_{t=1}^{T}(x_t)^2$$

- encourages small x

mean-square smooth

$$\phi(x) = \frac{1}{T-1}\sum_{t=1}^{T-1}(x_{t+1}-x_t)^2$$

- encourages smooth x

Boolean

$$\phi(x) = \begin{cases} 0 & x_t \in \{0,1\} \\ \infty & \text{otherwise} \end{cases}$$

- requires values 0 or 1

(we'll see more complex examples later)

Statistical interpretation

- assuming $Z = \int \exp -\phi(x)\, dx < \infty$, define density

$$p(x) = \frac{1}{Z} \exp -\phi(x)$$

- $\phi(x)$ is negative log-likelihood of x (plus constant)
- suppose
  - all classes have a density
  - $x^1, \ldots, x^K$ are independent random variables with densities $p_1, \ldots, p_K$
- then SD is the *maximum a posteriori* (MAP) estimate of components

- moving on, we won't focus on statistical framing

Class parameters

- class costs have *parameters* $\theta \in \Theta$, expressed as $\phi(x;\theta)$
- examples
  - scale a fixed function, *i.e.*, $\phi(x;\theta) = \theta\ell(x)$, $\theta > 0$
    (typically use symbol λ here)
  - specify constant values or constraints, *e.g.*, $\phi(x;\theta) = \mathcal{I}(\theta_1 \leq x \leq \theta_2)$, $\theta_1 \leq \theta_2$
  - specify a basis, *i.e.*, $\phi(x,z;\theta) = \mathcal{I}(x = \theta z)$, $\theta \in \mathbf{R}^{T \times d}$
    (sometimes called a *dictionary*, note helper variable $z \in \mathbf{R}^d$)

- parameters are used to change or shape the decomposition
- common practice: find decomposition for several values of parameters, then select best (more on that later)

Example: Sum-absolute small with transform

$$\phi(x; \lambda) = \lambda \|Dx\|_1$$

- $D \in \mathbf{R}^{r \times T}$; λ is a weight parameter
- encourages sparsity of Dx

- $D = I$: encourages sparse x (Laplacian prior)
- D is 1st order difference matrix: encourages sparse differences in x, *i.e.*, piecewise constant x
- D is 2nd order difference matrix: encourages sparse second differences, *i.e.*, piecewise affine x

Example: Monotonic with regularization

$$\phi(x;\lambda) = \begin{cases} \lambda\ell(x) & x_t \leq x_{t+1} \text{ for } t = 1, \ldots, T-1 \\ \infty & \text{otherwise} \end{cases}$$

- $\ell(x) : \mathbf{R}^T \to \mathbf{R} \cup \{\infty\}$ is some loss; λ is a weight parameter
- x cannot decrease

- $\ell(x) = \sum_t (x_{t+1} - x_t)^2$: encourages smooth (and monotone) x
- $\ell(x) = \sum_t |x_{t+2} - 2x_{t+1} + x_t|$: encourages piecewise affine (and monotone) x

Hold out validation

- select some entries of y randomly as 'test'' or 'hold out' set $\mathcal{T} \subset \mathcal{K}$
- find decomposition using entries $\mathcal{K} \setminus \mathcal{T}$ and impute held out entries $\widehat{y}_t$, $t \in \mathcal{T}$
- evaluate mean-square test error $\frac{1}{|\mathcal{T}|} \sum_{t \in \mathcal{T}} (y_t - \widehat{y}_t)^2$
- for more stable validation, can use cross validation

- validation guides choice of component losses and parameters, together with expert prior knowledge

Specifying signal decomposition in OSD

OSD: open source Python package for optimization-based signal decomposition

```
# residual component
c1 = SumSquare(weight=1/len(y))
# constant component
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# linear degradation component
c3 = Aggregate([NoCurvature(), FirstValEqual(0)])
# seasonal baseline component
c4 = Aggregate([SumSquare(weight=5e0, diff=2), Periodic(365),
               AverageEqual(0, period=365)])
# soiling component
c5 = Aggregate([Inequality(vmax=0), SumAbs(weight=1e-5),
               SumQuantile(weight=1e-5, diff=1, tau=0.9),
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problem = Problem(data=y, components=[c1, c2, c3, c4, c5])
```

- classes are predefined Python objects
- construct models by combining objects
- can carry out (cross) validation

Outline

Introduction

Optimization based signal decomposition

Solution methods

Example: Estimated soiling losses in solar generators

Solving SD problems

- we'll give the flavor of three solution methods
- all provably give a (globally) optimal decomposition when problem is convex
- or reasonable approximate decomposition when problem is not convex
- all use the approach of breaking a problem into smaller problems
- we'll assume that first component class is mean-square small

$$\phi_1(x) = \frac{1}{T}\|x\|_2^2$$

so we interpret x^1 as a residual

Block coordinate descent algorithm

$$\begin{array}{ll} \text{minimize} & \frac{1}{T}\|x^1\|_2^2 + \phi_2(x^2) + \cdots + \phi_K(x^K) \\ \text{subject to} & y_t = x_t^1 + \cdots + x_t^K, \quad t \in \mathcal{K} \end{array}$$

SD-BCD algorithm:

- minimize over x^1 and x^2, holding others constant
- then over x^1 and x^3, then over x^1 and x^4, ...
- continue cyclically in Gauss-Seidel fashion

SD-BCD is a feasible descent method, *i.e.*, iterates are feasible and objective decreases

Masked proximal operator

- minimizing over x^1 and x^i is evaluating the *masked proximal operator* of ϕ_i

$$\mathbf{mprox}_{\phi_i}(v) = \operatorname*{argmin}_x \left(\phi_i(x) + \frac{\rho}{2} \sum_{t \in \mathcal{K}} (x_t - v_t)^2 \right)$$

  for SD-BCD, $\rho = 2/T$
- *cf.* proximal operator of ϕ^i

$$\mathbf{prox}_{\phi_i}(v) = \operatorname*{argmin}_x \left(\phi_i(x) + \frac{\rho}{2} \sum_{t} (x_t - v_t)^2 \right)$$

- with no unknown entries, the two are identical

Alternating direction method of multipliers algorithm

SD-ADMM:

Initialize. Set $u^0 = 0 \in \mathbf{R}^q$, and $(x^i)^0 \in \mathbf{R}^T$, $i = 1, \ldots, K$, as some initial estimates
for iteration $j = 0, 1, \ldots$

1. *Evaluate masked proximal operators of component classes in parallel.*

$$(x^i)^{j+1} = \mathbf{mprox}_{\phi_k}((x^i)^j - 2\mathcal{M}^* u^j), \quad i = 1, \ldots, K.$$

2. *Dual update.*

$$u^{j+1} = u^j + \frac{1}{K}\left(\sum_{i=1}^{K} \mathcal{M}(x^i)^{j+1} - \mathcal{M}y\right).$$

- $\mathcal{M}z$ gives entries z_i, $i \in \mathcal{K}$, in some known order
- $\mathcal{M}^* u$ puts entries of u into known entries, and zeros in unknown entries

SD-BCD versus SD-ADMM

- both access component losses only via masked proximal operators
- both converge to an optimal decomposition when SD problem is convex

- for convex problems
  - $\rho = 2/T$ works well for both SD-BCD and SD-ADMM
  - SD-BCD is a bit faster than SD-ADMM

- for nonconvex problems
  - $\rho = 1.4/T$ gives good results for SD-ADMM
  - SD-ADMM tends to give better decompositions than SD-BCD

But . . . masked proximal operators can be difficult to evaluate

- consider class of smooth x bounded by 1

$$\phi(x) = \begin{cases} \sum_{t=1}^{T-2}(x_t - 2x_{t+1} + x_{t+2})^2 & \|x\|_\infty \leq 1 \\ \infty & \text{otherwise} \end{cases}$$

- simple and useful class with no closed-form **mprox** (or **prox**)
- but, can be expressed as sum of two functions with simple proximal operators

$$\phi(x) = \sum_{t=1}^{T-2}(x_t - 2x_{t+1} + x_{t+2})^2 + \mathcal{I}(\|x\|_\infty \leq 1) = f(x) + g(x)$$

- this is an example of a *quadratic-separable* (QS) function
- inspiration for third solution method

Quadratic-separable optimization

quadratic-separable (QS) optimization problem:

$$\begin{array}{ll} \text{minimize} & f(x) + g(x) \\ \text{subject to} & Ax = b \end{array}$$

- f is convex quadratic
- g is separable, $g(x) = g_1(x_1) + \cdots + g_n(x_n)$
- linear equality constraints

- solution via ADMM only requires $\mathbf{prox}_g$, which is straightforward

SD via QS optimization

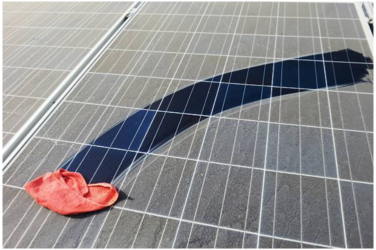
- when all ϕ_i are partial minimizations of QS functions

$$\phi(x) = \inf_z \{f(x,z) + g(x,z) \mid Ax + Bz = c\}$$

  SD problem is a QS problem
- complex class costs are broken into smaller parts
- separable functions with easy proximal operators are *atoms*
- these atoms are the basis of extensible modeling language

Outline

PV soiling



- build-up of material on the surface of PV modules over time
- can cause large yield reduction, as high as $-1\%/\text{day}$
- highly variable and difficult to predict
  - system geometry, local climate/weather, proximity to agriculture/industry,...
- important to industry (entire PVSC subarea, PVRW, *etc.*)

Soiling data

- we use NREL's soiling simulation model (Skomedal and Deceglie 2020)
- simulates daily PV energy including seasonal variation, long-term degradation, and soiling losses
- multiplicative loss model
- soiling component is known exactly, so we can validate SD

Data preprocessing

- take log of signal
- additive decomposition is multiplicative in original data
- min-max scaling to $[0, 10]$
- chosen to provide adequate dynamic range for soiling and degradation components

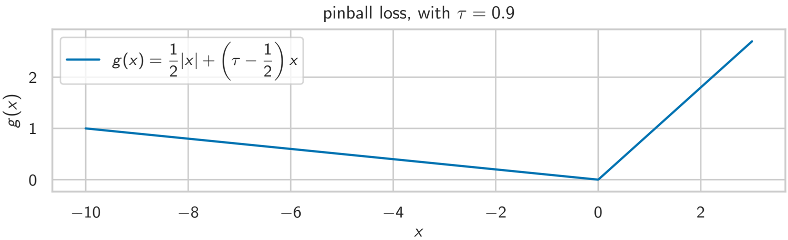
Component class losses

component	$\phi_i(x)$	description
1	$(1/T)\,\|x\|_2^2$	residual
2	$\mathcal{I}(D_1 x = 0)$	constant
3	$\mathcal{I}(D_2 x = 0)$	linear
4	$\lambda_3 \, \|D_2 x\|_2^2 + \mathcal{I}\,(x_t = x_{t+365})$	smooth & periodic
5	$\ell_{\mathrm{soil}}(x)$	soiling

Soiling class loss

$$\ell_{\text{soil}}(x) = \ell_1(x) + \ell_2(x) + \ell_3(x) + \ell_4(x)$$

	soiling loss term	description
ℓ_1	$\mathcal{I}(x \leq 0)$	non-positive
ℓ_2	$\lambda_{5a} \left\Vert x \right\Vert_1$	sparse
ℓ_3	$\lambda_{5b} \sum_{t=1}^{T-1} \left[\frac{1}{2}\left\vert (D_1 x)_t \right\vert + \frac{2}{5}(D_1 x)_t\right]$	asymmetric 1^{st} diff.
ℓ_4	$\lambda_{5c} \left\Vert D_2 x \right\Vert_1$	piecewise affine



Parameters

param.	value
λ_3	5
λ_{5a}	1×10^{-5}
λ_{5b}	5×10^{-3}
λ_{5c}	1×10^{-5}

- weights chosen to provide satisfactory results, not through holdout validation

SD code specification

```
# residual component
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problem = Problem(data=y, components=[c1, c2, c3, c4, c5])
```
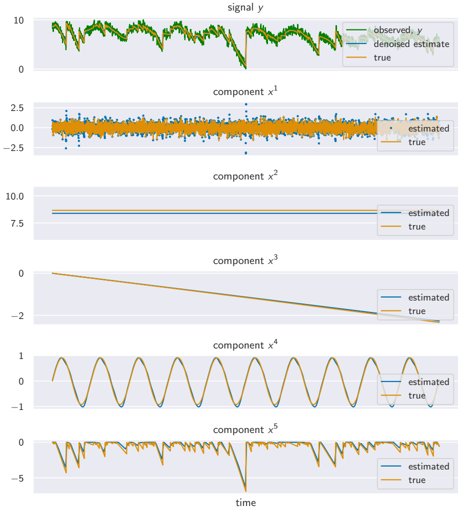

Results

- solved via QS algorithm
- solve time <10 seconds on 2016 MacBook Pro, no parallelization
  - $T = 3{,}653$
  - 40,543 variables
- components match true values very closely
- median daily soiling rate
  - estimated: $-0.071\%/\text{day}$
  - true: $-0.075\%/\text{day}$
- total annual degradation
  - estimated: $-0.48\%/\text{yr}$
  - true: $-0.50\%/\text{yr}$



Conclusions

- developed an SD framework
- user focus on component characteristics, not solution method
- we developed three custom, distributed solution methods that scale
- implemented a modeling language for SD
- embedded in Solar Data Tools
- already used my me and others on multiple PV data analysis problems

`https://github.com/cvxgrp/signal-decomposition`
`https://github.com/slacgismo/solar-data-tools`

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`https://bmeyers.github.io/about`

Appendix

Masking operator

- recall that equality constraint holds over known set
- introduce masking operator $\mathcal{M} : (\mathbf{R} \cup \{?\})^T \to \mathbf{R}^q$, where $q = |\mathcal{K}| \leq T$
- we also use its adjoint $\mathcal{M}^* : R^q \to R^T$, which sets unknown entries to zero
- note that while y can have missing values, $\mathcal{M}y$ does not
- for any $z \in (\mathbf{R} \cup \{?\})^T$, $\mathcal{M}^*\mathcal{M}z$ is z with unknown entries replaced with zeros

Stopping criterion

- last building block is the stopping criterion
- algorithms will be iterative, updating estimates until convergence
- let x^i_- be estimate of x^i before an iterate, and x^i_+ be the estimate after
- can express the optimality residual for unconstrained SD problem as

$$r = \left(\frac{1}{K-1} \sum_{i=2}^{K} \left\| \mathcal{M} \left(\rho(x^i_- - x^i_+) - \frac{2}{T} x^1 \right) \right\|_2^2 \right)^{1/2}$$

- if SD problem is convex and $r = 0$, components are optimal