Model Correction using a Nuclear Norm Constraint

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Motivation

We create mathematical models to simulate the operation of a real world or system.

Not surprisingly, the models will contain some error:
- simplifications for computational tractability
- linearization, numerical error
- boundary conditions or geometry
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Thinking outside the Box, some models can be made less wrong / more useful. This is the subject of today’s talk.
Problem Definition

Let \( \mathcal{F} : \mathbb{R}^n \rightarrow \mathbb{R}^m \) be “true” operator taking input \( x \in \mathbb{R}^n \) to observable space. Let \( d \in \mathbb{R}^m \) be an observation obtained as

\[
d = \mathcal{F}(x) + \epsilon
\]

where \( \epsilon \) represents measurement noise.

**Goal:** Formulate and solve a model correction optimization problem to recover an \( \mathcal{F} \) that is only partially specified. In this talk, assume \( A \) is known and

\[
\mathcal{F}(x) = A(x) + B(x).
\]

Model correction problem is to recover \( B \). Need additional constraints on \( B \) to obtain a well-posed optimization problem.
Motivating Test Problem

Discrete ill-posed problem (e.g. deblurring, Xray-CT)

\[ Ax = d + \epsilon. \]

If operator not known exactly model should be replaced by

\[(A + B)x = d + \epsilon.\]

While \( B \) is unknown, and in general \( x \) is unknown, we assume we can sample input space and have access to corresponding output realizations for each of the samples.
Sample Average Approximation

SAA\(^1\) : Expectation wrt the input space & the measurement noise approximated by a sample ave. est. of a random sample.

\[
\hat{B} = \arg\min_B \frac{1}{n_x n_\epsilon} \sum_{j=1, j=1}^{n_x, n_\epsilon} D \left( (A(x_i) + B(x_i)) - d_{ij} \right)
\]

subject to constraint on \(B\), \(n_x\) is the number of input draws, \(n_\epsilon\) is number of data realizations for each input realization.

**Problem** \((A(x) = Ax, B(x) = Bx, D(y) = \|y\|^2_2)\)

\[
\hat{B} = \arg\min_B \frac{1}{n_x n_\epsilon} \sum_{i=1, j=1}^{n_x, n_\epsilon} \|(A + B)x_i - d_{i,j}\|^2_2,
\]

subject to a structural constraint on \(B\).

Restrictions on Operator Structure

Many constraints on $B$ possible. Choose rank-based:

**Problem**

$$\hat{B} = \arg\min_B \| (A + B)X - D \|_F^2$$

$$\text{s.t. } \text{rank}(B) \leq \frac{\delta}{2}$$

Relax the constraint:

**Problem**

$$\hat{B} = \arg\min_B \| (A + B)X - D \|_F^2$$

$$\text{s.t. } \| B \|_* \leq \frac{\delta}{2}$$
Optimization Problem with Nuclear Norm Regularization

Several options for solving the optimization problem\textsuperscript{[1]}

- Interior Point Methods
- Alternating Direction Method of Multipliers (ADMM)
- Projected Sub-Gradient Method
- More recent work by Jaggi and Sulovsky: recast the optimization problem over positive semidefinite matrices with unit trace and then apply Hazan’s algorithm.

\textsuperscript{[1]}Hao, Horesh, & K., “Nuclear norm optimization and its application to observation model specification,” in Compressed Sensing and Sparse Filtering, 2014
Hazan’s Algorithm

Hazan’s Algorithm deals with problems of the form:

$$\min_{Z \in S} f(Z)$$

where $f$ is convex and $S$ is the set of all symmetric positive semidefinite $d \times d$ matrices with unit trace.

Each iteration involves the calculation of a single approximate eigenvector of a matrix of size of $d \times d$.

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Sparse approximation solutions to semidefinite programs by Hazan, E. 2008
Algorithm

From Jaggi and Sulovksy “A Simple Algorithm for Nuclear Norm Regularized Problem” 2010, for any non-zero matrix $B \in \mathbb{R}^{n \times m}$ and $\delta \in \mathbb{R}$:

$$\|B\|_* \leq \frac{\delta}{2} \iff \exists \text{ symmetric } M, N \text{ s.t.}$$

\[
\begin{pmatrix}
M & B \\
B^T & N
\end{pmatrix} \succeq 0
\]

and

$$\text{Tr}(M) + \text{Tr}(N) = \delta.$$
Steps

Let $Z = \begin{pmatrix} M & B \\ B^T & N \end{pmatrix}$.

- Define $\hat{f}(Z) = f(B) = \| (A + B)X - D \|_F^2$.
- Want to solve
  \[
  \min_Z \hat{f}(Z)
  \]
  s.t. $Z \in S^{(m+n) \times (m+n)}$, $Z \succeq 0$, $\text{Tr}(Z) = \delta$

- Scale all matrix entries by $\frac{1}{\delta}$
- Apply Hazan’s algorithm, then unscale
Algorithm

Input: \( f, v_0 \in \mathbb{R}^{(m+n) \times 1} \) with \( ||v_0|| = 1 \); scaled matrices

Initialize: \( Z_1 = v_0v_0^T \)

for \( k = 1 \) until convergence do

Extract \( B_k = Z_k(1 : m, m+1 : m+n) \)

Compute \( \nabla f_k := ((A + B_k)X - D)X^T \)

We have \( \nabla \hat{f}_k := \begin{pmatrix} 0 & \nabla f_k \\ \nabla f_k^T & 0 \end{pmatrix} \)

Compute \( v_k := \text{eigs}(-\nabla \hat{f}_k, 1, LA') \)

Line search for step length \( a_k \)

Update \( Z_{k+1} = Z_k + a_k(v_kv_k^T - Z_k) \)

end for

Return \( \hat{B} = \delta \cdot Z(1 : m, m+1 : m+n) \)
Numerical Examples

- Mimic the semi-blind deconvolution problem, only an approximation to blurring operator is known a-priori.
- 100 MR images from the Auckland MRI Research group database.
- Pre-process the images by cropping the watermark and resizing the cropped images to the size of $55 \times 55$.
- Randomly choose 80 images (sampled integers from 1:100 uniformly) to serve as the training set and 20 of remainder as the test set.

http://atlas.scmr.org/download.html
Example 1

- Let $T(b_w, \sigma)$ be symmetric, doubly block Toeplitz matrix $T$ that models blurring of an image by a Gaussian point spread function; $b_w, \sigma$ control (block) bandwidth and blur.
- $A = T(4, 4)$
- $B$ defined from singular triples of $T(3, 2)$ numbered 110 to 120.
- Compute $D = (A + B)X + N$ where $N$’s columns have zero mean, white Gaussian noise such that the noise to signal ratio for all measured data is .5 percent.
- Run 120 iterations. Compare the best TSVD regularized solutions using the SVDs of $A, A + B, A + \hat{B}$. 
True Blurred Training Images
\[ AX \text{ vs } (A + B)X \]
Rel. Errors, TSVD recons, 20 from test set
Example 1, Test Slice 16
Rel. Errors after 400 iterations
Enforcing Different Structure

What if \( B(x) \neq Bx \), but rather \( B(x) = K[B]x \)?

Example [Kamm & Nagy, 1998] Let \( v \) be of length \( n \), \( n \) odd, \( \text{toep}(v) \) creates an \( n \times n \) banded Toeplitz matrix with \( v(\frac{n+1}{2}) \) as the diagonal entry:

\[
\text{toep} \left( \begin{bmatrix} a \\ b \\ c \end{bmatrix} \right) = \begin{bmatrix} b & a & 0 \\ c & b & a \\ 0 & c & b \end{bmatrix}
\]
Additional Structure from $B$

Given $n \times n$ $B$, make a BTTB matrix from blocks $\text{toep}B(:,i)$ in a similar manner.

For $B$ with 3 columns:

$$K[B] = \begin{bmatrix}
\text{toep}(B(:,2)) & \text{toep}(B(:,1)) & 0 \\
\text{toep}(B(:,3)) & \text{toep}(B(:,2)) & \text{toep}(B(:,1)) \\
0 & \text{toep}(B(:,3)) & \text{toep}(B(:,2))
\end{bmatrix}.$$
Convexity, Constraint Revisited

It is possible to show that
\[ K[B]x = K[\text{reshape}(x, n, n)]\text{vec}(B). \]

So,
\[ \sum \|Ax_{ij} + B(x_{ij}) - d_{ij}\|_F^2 \]
still convex in entries of \( B \)

Significance of the (ideal) rank-based constraint on \( B \):

\[ B = \sum_{i=1}^{k} \sigma_i u_i v_i^T \Rightarrow K[B] = \sum_{i=1}^{k} \text{toep}(\sqrt{\sigma_i} v_i) \otimes \text{toep}(\sqrt{\sigma_i} u_i), \]

Algorithm now cheap - matrix of partials is now \( n \times n \), matvecs with FFTs.
Example 2

- $A = T(10, 4)$
- $B = T(7, 3.1) + T(4, 2.2) + T(5, 3.5)$
- Same testing setup as before (random selection of 80 images) and testing on the remainder, Gaussian $\frac{1}{2}$ percent noise added (once per test image).
Relative Squared Convergence Error

![Graph showing relative squared convergence error over iterations and squared relative errors.](image)
Difference in Data Space: \[ |BX_{train}| \]
Difference in Data Space: $| (B - \hat{B}) X_{train} |$
Errors on 20 Test Data

\[
\frac{\|AX-(A+B)X\|_F}{\| (A+B)X \|_F} \quad \text{vs.} \quad \frac{\| (\hat{B}-B)X \|_F}{\| (A+B)X \|_F}
\]
One Extension to Tensors

$B$ is order $> 2$ tensor from which we define $K[B](x)$.

$B \in \mathbb{R}^{n \times n \times n}$, $B = \sum_{i=1}^{r} u_i \circ v_i \circ w_i \Rightarrow K[B]$ to a sum of 3-way Kronecker products of structured matrices


But what do we mean by $\|B\|_\star$?
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More thinking outside the Box....
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But what do we mean by $\|B\|_*$?

Use $\|B\|_{\text{TNN}}$ definition [Hao, 2014] based on tSVD [K. & Martin, 2011].
Current & Future Work

Other examples (PDEs) (thanks: Raya Horesh, IBM Watson)
Current & Future Work

- Tensors
- Other examples (PDES)
- Other choices for $\mathcal{D}$
- Investigate other possible constraints on the operator (nonlinear correction).