# COMPUTATIONAL METHODS IN APPLIED INVERSE PROBLEMS 

Uri Ascher

Department of Computer Science<br>University of British Columbia<br>October 2017

## Four Lectures

- Calibration and simulation of deformable objects
- Data manipulation and completion
- Estimating the trace of a large implicit matrix and applications
- Numerical analysis in visual computing: not too little, not too much


## Outline

- Motivation
- Completing scarce (sparse) data
- Uncertainty in data locations
- Forced to cut corners
- Randomized algorithms for many data sets
- Conclusions


## Here is the T-shirt

## When All Else Fails manipulate the data

## Data completion and manipulation

- The practice of manipulating given observed data for solving inverse problems is known to have its perils: loss of statistical relevance, danger of calibrating a model to handle our own generated errors, etc.

Completing scarce data" by some interpolation/extrapolation or other approximation
Preferring to see data given at regular mesh nodes, or otherwise having
a hidden uncertainty in the location of data values
"Completing data" to obtain a more efficient algorithm
"Completing data" to obtain a "more solid theory"
(5) Manipulating data because we don't know how to solve the problem otherwise.

## DATA COMPLETION AND MANIPULATION

- The practice of manipulating given observed data for solving inverse problems is known to have its perils: loss of statistical relevance, danger of calibrating a model to handle our own generated errors, etc.
- And yet it seems to be everywhere in practice!
(1) "Completing scarce data" by some interpolation/extrapolation or other approximation
(2) Preferring to see data given at regular mesh nodes, or otherwise having a hidden uncertainty in the location of data values
(3 "Completing data" to obtain a more efficient algorithm
(1) "Completing data" to obtain a "more solid theory"
(0) Manipulating data because we don't know how to solve the problem otherwise.
- When is it OK to do this?!
- Attempt to get more insight by considering case studies.


## DATA COMPLETION AND MANIPULATION

- The practice of manipulating given observed data for solving inverse problems is known to have its perils: loss of statistical relevance, danger of calibrating a model to handle our own generated errors, etc.
- And yet it seems to be everywhere in practice!
(1) "Completing scarce data" by some interpolation/extrapolation or other approximation
(2) Preferring to see data given at regular mesh nodes, or otherwise having a hidden uncertainty in the location of data values
(3) "Completing data" to obtain a more efficient algorithm
(4) "Completing data" to obtain a "more solid theory"
(5) Manipulating data because we don't know how to solve the problem otherwise.
- When is it OK to do this?!
- Attempt to get more insight by considering case studies.


## OUR CASE STUDIES

(1) Inverting Maxwell's equations and DC resistivity in exploration geophysics
[Haber, A. \& Oldenburg, 2004]
(2) Recovering local volatility surface in financial mathematics [Albani, A., Yang \& Zubelli, 2017; A., A. \& Z., 2017]
(3) Denoising of surface triangle mesh [Huang \& A., 2008]
(a) Calibrating and simulating soft bodies in computer graphics [Wang, Wu, Yin, A., Liu \& Huang, 2015]
(6) Obtaining union of observation locations for many data sets [Roosta-Khorasani, van den Doel \& A., 2014]

## Inverse problem setting

- Given observed data $\mathbf{d} \in \mathbb{R}^{\prime}$ and a forward operator $\mathbf{f}(m)$ which provides predicted data for each instance of distributed parameter function $m$, find $m$ (discretized and reshaped into $m$ ) such that the predicted and observed data agree to within noise:

$$
\mathbf{d}=\mathbf{f}(\mathbf{m})+\boldsymbol{\eta}
$$

- Consider a case where a PDE must be solved to evaluate the forward operator, i.e., $\mathbf{f}(\mathbf{m})=P \mathbf{u}=P G(\mathbf{m}) \mathbf{q}$, where $G$ is a discrete Green's function.
- Iterative algorithm on $m$ to reduce objective. Assuming $\eta \sim \mathcal{N}\left(0, \sigma^{2} l\right)$, the maximum likelihood (ML) data misfit function is


## Inverse problem setting

- Given observed data $\mathbf{d} \in \mathbb{R}^{\prime}$ and a forward operator $\mathbf{f}(m)$ which provides predicted data for each instance of distributed parameter function $m$, find $m$ (discretized and reshaped into $m$ ) such that the predicted and observed data agree to within noise:

$$
\mathbf{d}=\mathbf{f}(\mathbf{m})+\boldsymbol{\eta}
$$

- Consider a case where a PDE must be solved to evaluate the forward operator, i.e., $\mathbf{f}(\mathbf{m})=P \mathbf{u}=P G(\mathbf{m}) \mathbf{q}$, where $G$ is a discrete Green's function.
- Iterative algorithm on $\mathbf{m}$ to reduce objective. Assuming $\eta \sim \mathcal{N}\left(0, \sigma^{2} l\right)$, the maximum likelihood (ML) data misfit function is

$$
\phi(\mathbf{m})=\|\mathbf{f}(\mathbf{m})-\mathbf{d}\|_{2}^{2}
$$

The discrepancy principle yields the stopping criterion

## Inverse problem setting

- Given observed data $\mathbf{d} \in \mathbb{R}^{\prime}$ and a forward operator $\mathbf{f}(m)$ which provides predicted data for each instance of distributed parameter function $m$, find $m$ (discretized and reshaped into $m$ ) such that the predicted and observed data agree to within noise:

$$
\mathbf{d}=\mathbf{f}(\mathbf{m})+\boldsymbol{\eta}
$$

- Consider a case where a PDE must be solved to evaluate the forward operator, i.e., $\mathbf{f}(\mathbf{m})=P \mathbf{u}=P G(\mathbf{m}) \mathbf{q}$, where $G$ is a discrete Green's function.
- Iterative algorithm on $\mathbf{m}$ to reduce objective. Assuming $\eta \sim \mathcal{N}\left(0, \sigma^{2} I\right)$, the maximum likelihood (ML) data misfit function is

$$
\phi(\mathbf{m})=\|\mathbf{f}(\mathbf{m})-\mathbf{d}\|_{2}^{2}
$$

The discrepancy principle yields the stopping criterion

$$
\phi(\mathbf{m}) \leq \rho, \quad \text { where } \rho=\sigma^{2} /
$$

## Outline

- Motivation
- Completing scarce (sparse) data
- Uncertainty in data locations
- Forced to cut corners
- Randomized algorithms for many data sets
- Conclusions


## Example (CS1): scarce data in ELECTROMAGNETIC DATA INVERSION

$G$ is Green's function for Maxwell's equations in time or frequency domain, $\mathbf{m}$ is conductivity or resistivity. [Haber, A. \& Oldenburg, 2004]


## EM DATA INVERSION IN GEOPHYSICS

Use Tikhonov-type regularization: a prior penalizing lack of smoothness in surface function $m$ through gradient.


Top: misfit. Bottom: recovered m.

## DUPIRE'S EQUATION (CS2)

[Dupire, 1994]: replace the Black-Scholes equation for option price by a parabolic PDE of the form

$$
\frac{\partial C}{\partial \tau}=\frac{1}{2} \sigma^{2}(\tau, K) K^{2} \frac{\partial^{2} C}{\partial K^{2}}-b K \frac{\partial C}{\partial K}, \quad \tau>0, K \geq 0
$$

s.t. initial and boundary conditions (for calls)

$$
\begin{aligned}
C(\tau=0, K)= & \left(S_{0}-K\right)^{+} \\
\lim _{K \rightarrow \infty} C(\tau, K)=0, \quad & \lim _{K \rightarrow 0} C(\tau, K)=S_{0}
\end{aligned}
$$

Here $\tau$ is time to maturity, $K$ is strike price, $C=C(\tau, K)$ is value of the European call option with expiration date $T=\tau$, and $\sigma(\tau, K)$ is volatility. Can write all this in operator form as

$$
\tilde{L}(\sigma) C=\tilde{q}\left(S_{0}\right)
$$

with $\tilde{L}$ a linear differential operator for a given $\sigma$.
Assume first that the stock price $S_{0}$ is a given parameter.
Calibrating the model: solve inverse problem for $\sigma(\tau, K)$ given $\sum_{\equiv} C$-data,

## Changing variables: LOG moneyness

To simplify and make problem dimensionless, change $K$ to $y=\log \left(K / S_{0}\right)$ (so $-\infty<y<\infty)$, then $u(\tau, y)=C\left(\tau, S_{0} \exp (y)\right) / S_{0}$ and $m(\tau, y)=\frac{1}{2} \sigma(\tau, K(y))^{2}$. Obtain

$$
-\frac{\partial u}{\partial \tau}+m\left(\frac{\partial^{2} u}{\partial y^{2}}-\frac{\partial u}{\partial y}\right)+b \frac{\partial u}{\partial y}=0, \quad \tau>0, y \in \Re,
$$

s.t. side conditions

$$
\begin{aligned}
u(\tau=0, y) \quad & =(1-\exp (y))^{+} \\
\lim _{y \rightarrow \infty} u(\tau, y)=0, & \lim _{y \rightarrow-\infty} u(\tau, y)=1 .
\end{aligned}
$$

Can write this as $L(m) u=q$.
Discretize over a mesh with step sizes $\Delta \tau$ and $\Delta y$; denote the corresponding discretization as

$$
L_{h}(m) u_{h}=q_{h} .
$$

## EXAMPLE: LOCATIONS OF (REAL) DATA

Locations of $u$-data values for the PBR data set.


## EXAMPLE: LOCATIONS OF (REAL) DATA

Locations of $u$-data values for the SPX data set.


## Interpolating/Extrapolating the data

- Several researchers have applied interpolation/extrapolation to this type of data, followed by assimilation of the resulting data set with the discretized Dupire PDE problem.
- Use [Kahale, 2005] for this purpose. This algorithm applies data completion with a "financial prior", insisting that the resulting data surface reproduce the "smile" effect.



## Interpolating/Extrapolating the data

- Several researchers have applied interpolation/extrapolation to this type of data, followed by assimilation of the resulting data set with the discretized Dupire PDE problem.
- Use [Kahale, 2005] for this purpose. This algorithm applies data completion with a "financial prior", insisting that the resulting data surface reproduce the "smile" effect.
- An obvious objection, however, is that the resulting data surface does not satisfy the discretized differential problem for any $m(\tau, y)$, and vice versa. The assimilation of these two pieces of information may be more difficult.
- Compare this to not modifying the given data, using for both cases a Tikhonov-type regularization as well as EnKF.


## Regularized inverse problem

- Maximum likelihood for simplest case of white noise:

$$
\phi\left(m_{h}, u_{h}\right)=\left\|P u_{h}-\mathbf{d}\right\|^{2}=\left\|P L_{h}\left(m_{h}\right)^{-1} q_{h}-\mathbf{d}\right\|^{2}
$$

where matrix $P$ projects to data locations: $P$ has many more columns than rows for original data, whereas $P=I$ for completed data.

- Regularize the problem: minimize the maximum a posteriori (MAP) merit function

$$
\phi_{R}\left(m_{h}, u_{h}\right)=\phi\left(m_{h}, u_{h}\right)+R\left(m_{h}\right)
$$

- Our Tikhonov-like regularization operator is ( $a_{0}$ a known constant)

$$
\begin{aligned}
R\left(m_{h}\right) & =\alpha_{1} \sum_{i} \sum_{j}\left(m_{i, j}-a_{0}\right)^{2} \\
& +\frac{\alpha_{2}}{\Delta \tau^{2}} \sum_{j} \sum_{i=1}^{M_{\tau}}\left(m_{i, j}-m_{i-1, j}\right)^{2}+\frac{\alpha_{3}}{\Delta y^{2}} \sum_{i} \sum_{j=1}^{M_{y}}\left(m_{i, j}-m_{i, j-1}\right)^{2}
\end{aligned}
$$

## Results for SPX data

Set $\alpha_{1}>0$ and compare working with the given sparse data vs using data completion by the Kahale algorithm.




## Conclusion for case study CS2

- These results clearly show that the data completion approach has not delivered.

> Additional tests for Henry Hub and WTI prices, using bilinear interpolation for the data completion and different $\alpha$-weights in the Tikhonov-type priors, also clearly indicate that it is better to avoid the extensive data completion required here: the market implied smile, which has an important relationship with market risk, is better fitted upon using just the original data. Both EnKF algorithms we tried Ernst \& Somersalo 2014] were trivially (and significantly) impro
adding additional regularization using $a_{0}$ and first derivatives. After this improvement the EnKF algorithms were comparable to but parameter search was required

## Conclusion for case study CS2

- These results clearly show that the data completion approach has not delivered.
- Additional tests for Henry Hub and WTI prices, using bilinear interpolation for the data completion and different $\alpha$-weights in the Tikhonov-type priors, also clearly indicate that it is better to avoid the extensive data completion required here: the market implied smile, which has an important relationship with market risk, is better fitted upon using just the original data.



## Conclusion for case study CS2

- These results clearly show that the data completion approach has not delivered.
- Additional tests for Henry Hub and WTI prices, using bilinear interpolation for the data completion and different $\alpha$-weights in the Tikhonov-type priors, also clearly indicate that it is better to avoid the extensive data completion required here: the market implied smile, which has an important relationship with market risk, is better fitted upon using just the original data.
- Both EnKF algorithms we tried [Iglesias, Law \& Stuart, 2013; Calvetti, Ernst \& Somersalo 2014] were trivially (and significantly) improved by adding additional regularization using $a_{0}$ and first derivatives.
- After this improvement the EnKF algorithms were comparable to but not better than the Tikhonov-type regularization. Big plus: no ad hoc parameter search was required.


## Outline

- Motivation
- Completing scarce (sparse) data
- Uncertainty in data locations
- Forced to cut corners
- Randomized algorithms for many data sets
- Conclusions


## ExAmples

The notion that a (potentially noisy) data value $d_{i}$ is given at a known, deterministic location $\mathbf{x}_{i}$ is often violated in practice. Here are some examples:

- Surface triangle mesh denoising [Huang \& A., 2008]
- Minimal prospectivity mapping [Granek \& Haber, 2014] (not considered further)
- Local volatility surface with uncertainty in price $S_{0}$ [Albani, A., Yang \& Zubelli, 2015]


## Typical image denoising (CS3)



Left: noisy image: noisy data at precisely prescribed pixel locations. Right: exact (ideally denoised?) image.

## Surface triangle mesh denoising



Left: noisy triangle mesh: the data are nodal values $\left(x_{i}, y_{i}, z_{i}\right)$. No distinction between data value and location! Uncertainty in higher dimension.
Right: Our denoised triangle mesh.
[We had set out to generalize multiscale techniques for image denoising and ended up devising a completely different multiscale method for the surface mesh.

## Surface triangle mesh denoising



Left: noisy triangle mesh: the data are nodal values $\left(x_{i}, y_{i}, z_{i}\right)$. No distinction between data value and location! Uncertainty in higher dimension.
Right: Our denoised triangle mesh.
[We had set out to generalize multiscale techniques for image denoising and ended up devising a completely different multiscale method for the surface mesh.]

## 3D SURFACE TRIANGLE MESH



Uncertainty in data locations triangle mesh vs image denoising

## Scanned noisy model (25K verts)


triangle mesh vs image denoising
Smoothed by MSAL


## Uncertainty in $S_{0}(\mathrm{CS} 2)$

- Recall Dupire's equation

$$
\begin{gathered}
\frac{\partial C}{\partial \tau}=\frac{1}{2} \sigma^{2}(\tau, K) K^{2} \frac{\partial^{2} C}{\partial K^{2}}-b K \frac{\partial C}{\partial K}, \quad \tau>0, K \geq 0 \\
C(\tau=0, K)=\left(S_{0}-K\right)^{+} \\
\lim _{K \rightarrow \infty} C(\tau, K)=0, \quad \lim _{K \rightarrow 0} C(\tau, K)=S_{0}
\end{gathered}
$$

But now, stock price $S_{0}$ has (well-quantified) uncertainty, as it is typically some average of daily prices.

- $\Rightarrow$ Add a term $\alpha_{5}\left(S_{0}-\hat{S}_{0}\right)^{2}$ to regularization prior $R=R\left(m_{h}, S_{0}\right)$, where $S_{0}$ is now random variable with measured mean (say) $\hat{S}_{0}$.


## Uncertainty in $S_{0}$ cont.

- Furthermore, recall that upon changing variables to log moneyness

$$
y=\log \left(K / S_{0}\right)\left(\text { also } u(\tau, y)=C\left(\tau, S_{0} \exp (y)\right) / S_{0}\right.
$$ $\left.m(\tau, y)=\frac{1}{2} \sigma(\tau, K(y))^{2}\right)$, obtain the nicer PDE

$$
-\frac{\partial u}{\partial \tau}+m\left(\frac{\partial^{2} u}{\partial y^{2}}-\frac{\partial u}{\partial y}\right)+b \frac{\partial u}{\partial y}=0, \quad \tau>0, y \in \Re
$$

Now the uncertainty in $S_{0}$ has moved into the independent variable $y$ !

- $\Rightarrow$ In addition to adding a term $\alpha_{5}\left(S_{0}-\hat{S}_{0}\right)^{2}$ to $R=R\left(m_{h}, S_{0}\right)$, update also

$$
\begin{aligned}
\phi\left(m_{h}, S_{0}\right) & =\alpha_{0} \sum_{i=1}^{l}\left(\left(P\left(S_{0}\right) L_{h}\left(m_{h}\right)^{-1} q_{h}\left(S_{0}\right)\right)_{i}-d_{i}\right)^{2} \\
& +\alpha_{4} \sum_{j=1}^{M_{y}}\left(\left(1-\exp \left(y_{j}\left(S_{0}\right)\right)\right)^{+}-\left(1-\exp \left(y_{j}\left(\hat{S}_{0}\right)\right)\right)^{+}\right)^{2}
\end{aligned}
$$

(In practice set $\alpha_{5}=0$.)

## Uncertainty in $S_{0}$ cont.

- Splitting method: Alternately freeze $S_{0}$ and $m_{h}$ while solving for the other one.
- This converges fast because of the weak coupling, even when using the variable $y$.
- In preliminary experiments we see roughly a $1-2 \%$ change in adjusted price.


## Outline

- Motivation
- Completing scarce (sparse) data
- Uncertainty in data locations
- Forced to cut corners?
- Randomized algorithms for many data sets
- Conclusions


## ExAmples

In some cases, it has been claimed that data completion/manipulation allows obtaining better results. Here are some examples:

- Matrix and tensor completion for seismic applications [da Silva \& Herrmann, 2015; da Silva PhD thesis, 2017]
- Motion calibration and simulation of a soft body [Wang, Wu, Yin, A., Liu \& Huang, 2015]


## EXAMPLE: FULL WAVEFORM INVERSION

Herrmann: use data completion of velocity field in order to solve this problem.


## Motion capture And CALIBRATION (CS4)

- Physically-based deformation modelling in Computer Graphics
- Want to simulate and animate motion of a soft body, such as a plant under wind or water pressure, cloth, steak, face, etc.
- Can model by elastodynamics and porous media, but need to calibrate the model.
- Do that calibration by fitting example data obtained by sensor hardware: motion capturing and tracking.

[Wang, Wu, Yin, A., Liu \& Huang; siggraph '15]


## Capturing data

Left: three Kinect sensors are placed around the object; Right: the deformation point cloud sequence is captured at 30 Hz .


## CAPTURING DATA CONT.

Left: a (high resolution) surface mesh $\mathbb{S}$ with 15,368 vertices is used as a template to track captured point clouds; Right: its (low resolution) corresponding volumetric mesh $\mathbb{T}$ with 9,594 nodes is used for spatial co-rotated linear FEM simulations.


## ELASTIC DEFORMATION

- Denote reference shape by $\mathbf{X}$ and dynamic, deformed positions at a time instant $t$ by $\mathbf{x}=\mathbf{x}(t)$.
- Element-wise stress-strain relationship using Hooke's law and Cauchy's linear strain tensor is

$$
\sigma=\mathbf{E}_{\epsilon}=\mathbf{E B}_{\mathbf{e}}\left(\mathbf{x}_{\mathbf{e}}-\mathbf{X}_{\mathbf{e}}\right)
$$

where the $6 \times 12$ matrix $\mathbf{B}_{\mathbf{e}}=\mathbf{B}_{\mathbf{e}}\left(\mathbf{X}_{\mathbf{e}}\right)$ depends on $\mathbf{X}_{\mathbf{e}}$ nonlinearly.

- For isotropic materials the $6 \times 6$ matrix $\mathbf{E}$ only depends on Young's modulus $E$ and Poisson's ratio $\nu$.
- Denoting the per-element rotation matrix obtained from polar decomposition by $\mathbf{R}_{\mathbf{e}}=\mathbf{R}_{\mathbf{e}}\left(\mathbf{x}_{\mathbf{e}}(t), \mathbf{X}_{\mathbf{e}}\right)$, the element-wise elastic forces using the co-rotated linear approximation are

$$
\begin{aligned}
\mathbf{f}_{\mathbf{e}}\left(E, \nu, \mathbf{X}_{\mathbf{e}}, \mathbf{x}_{\mathbf{e}}(t)\right) & =\mathbf{R}_{\mathrm{e}} \mathbf{K}_{\mathbf{e}}\left(\mathbf{R}_{\mathrm{e}}^{\top} \mathbf{x}_{\mathbf{e}}(\mathbf{t})-\mathbf{X}_{\mathbf{e}}\right), \\
\mathbf{K}_{\mathbf{e}} & =V_{e} \mathbf{B}_{\mathrm{e}}^{\top} \mathbf{E} \mathbf{B}_{\mathbf{e}},
\end{aligned}
$$

$\mathrm{K}_{\mathrm{e}}$ is $12 \times 12$ element stiffness matrix and $V_{e}$ is element volume.

## EQUATIONS OF MOTION

- Assemble force contributions from all FEM elements
- Summon Newton's 2nd law: at time $t$

$$
\mathbf{M} \ddot{\mathbf{x}}+\mathbf{D} \dot{\mathbf{x}}+\hat{\mathbf{K}} \mathbf{x}=(\mathbf{R K}) \mathbf{X}+\mathbf{f}_{\mathrm{ext}}, \quad \hat{\mathbf{K}}=\mathbf{R} \mathbf{K R}^{\boldsymbol{\top}} .
$$

- Stiffness matrix $\hat{\mathbf{K}}$ is sparse and is assembled from element contributions. Mass matrix $\mathbf{M}$ is lumped.
- Use Rayleigh damping: $\mathbf{D}=\alpha \mathbf{M}+\beta \hat{\mathbf{K}}$.
- Model calibration parameters in simplest case are

$$
\mathbf{p}=(E, \nu, \alpha, \beta), \quad \text { so } \mathbf{m}=(\mathbf{p}, \mathbf{X}) .
$$

Often have more than one control point, for each of which there is a Young modulus.

## Motion TrACKING AND INVERSE PROBLEM

- Motion tracking: physically-based probabilistic tracking: for given $\mathbf{p}$ and $\mathbf{X}$, find captured trajectory $\mathbf{x}=\hat{\mathbf{x}}_{t}$.
- This tracking problem involves an inference (EM) algorithm.
- Inverse problem: deformation parameter estimation:

$$
\min _{\mathbf{p}, \mathbf{x}} \sum_{t}\left\|\mathbf{x}_{t}-\hat{\mathbf{x}}_{\mathbf{t}}\right\|^{2} .
$$



## Data manipulation to the rescue

- Employ a splitting method between $\mathbf{p}$ and $\mathbf{X}$. Fortunately this works very well because of weak coupling between these unknown groups.
- Use Nelder-Mead for $\mathbf{p}$ as there are many local minima. However, this is good only for a few unknowns.
- Many more nontrivial details are described in the paper.
- Nice looking results are obtained! see the videos and a separate talk.
- However, the calibration (parameter estimation) part of the process uses manufactured data.


## DATA MANIPULATION TO THE RESCUE

- Employ a splitting method between $\mathbf{p}$ and $\mathbf{X}$. Fortunately this works very well because of weak coupling between these unknown groups.
- Use Nelder-Mead for $\mathbf{p}$ as there are many local minima. However, this is good only for a few unknowns.
- Many more nontrivial details are described in the paper.
- Nice looking results are obtained! see the videos and a separate talk.
- However, the calibration (parameter estimation) part of the process uses manufactured data.
- Attempts to estimate the parameters directly from the point cloud data have not worked out well


## Outline

- Motivation
- Completing scarce (sparse) data
- Uncertainty in data locations
- Forced to cut corners
- Randomized algorithms for many data sets
- Conclusions


## Inverse problem with s data sets (CS5)

After discretization and for our problems of interest:

$$
\begin{aligned}
\mathbf{d}_{i} & =\mathbf{f}_{i}(\mathbf{m})+\boldsymbol{\eta}_{i}, \quad i=1,2, \ldots, s \\
\mathbf{f}_{i}(\mathbf{m}) & =P \mathbf{u}_{i}=P G(\mathbf{m}) \mathbf{q}_{i}
\end{aligned}
$$

## Calculating " $G(\mathbf{m}) \mathbf{q}_{i}$ " for each $i$ is costly!

- $\mathbf{d}_{i} \in \mathbb{R}^{\prime}$ is the measurement obtained in the $i^{t h}$ experiment
- $\mathbf{f}_{i}$ is the known forward operator for the $i^{\text {th }}$ experiment
- $\boldsymbol{m} \in \mathbb{R}^{/ m}$ is the sought-after model
- $\boldsymbol{\eta}_{i}$ is the noise incurred in the $i^{\text {th }}$ experiment
- $s$ is the total number of experiments
- $\mathbf{u}_{i} \in \mathbb{R}^{\prime / u}$ is the $i$ th field
- $\mathbf{q}_{i} \in \mathbb{R}^{\prime / u}$ is the $i$ th source
- $G^{-1}$ is a square matrix discretizing the PDE with the $B C$
- $P=P_{i}$ is the projection matrix for the $i^{t h}$ experiment


## Application: DC resistivity

- PDE with multiple sources

$$
\begin{aligned}
& \nabla \cdot\left(\mu(\mathbf{x}) \nabla u_{i}\right) \quad=\quad q_{i}, \quad i=1, \ldots, s \\
& \left.\frac{\partial u_{i}}{\partial \nu}\right|_{\partial \Omega}=0
\end{aligned}
$$

- Conductivity $\mu(\mathbf{x})$ is expressed as a point-wise function of $m(\mathbf{x})$ (e.g., use tanh to incorporate known bounds on $\mu$ ).
- The operator $G(\mathbf{m})$ is the inverse of the above PDE discretized on a staggered grid.
- Use different selections of sources $q_{i}$, yielding corresponding fields $u_{i}$.
- Data is measured only on part of the domain's boundary.
- Use any prior we may have for this very difficult problem!


## DC RESISTIVITY EXPERIMENT SETUP

- Domain $\Omega$ is the unit square. Sources are of the form

$$
q_{i}(\mathbf{x})=\delta\left(\mathbf{x}-\mathbf{x}_{1}^{i}\right)-\delta\left(\mathbf{x}-\mathbf{x}_{2}^{i}\right)
$$

with $\mathbf{x}_{1}$ positive unit point source on west boundary, $\mathbf{x}_{2}$ negative unit point source on east boundary. Vary $p$ boundary wall locations to get $s=p^{2}$ data sets.

- Receivers are all grid points on north and south walls. No sources or receivers at corners.
- Uniform $64 \times 64$ mesh
- For bounds set $\mu_{\text {max }}=1.2 \max \mu(\mathbf{x}), \mu_{\text {min }}=1.2^{-1} \min \mu(\mathbf{x})$
- PCG inner iteration limit $r=20$; cgtol $=1$.e-3.


## Example: $\mu_{I}=.1, \mu_{I I}=1, \mu_{I I}=.01$, noISe $2 \%$


(a) True model

(b) $s=3,969$

(c) $\mathrm{s}=49$

- Thus, we want $s$ larger for better reconstruction quality.
- But the cost of solving the problem grows very fast! (at least linearly with s). Need to find more efficient approximations for evaluating misfit function $\phi(\mathbf{m})$.


## Example: $\mu_{I}=.1, \mu_{I I}=1, \mu_{I I}=.01$, noISe $2 \%$


(d) True model

(e) $\boldsymbol{s}=3,969$

(f) $s=49$

- Thus, we want $s$ larger for better reconstruction quality.
- But the cost of solving the problem grows very fast! (at least linearly with $s$ ). Need to find more efficient approximations for evaluating misfit function $\phi(\mathbf{m})$.


## Monte Carlo to approximate the misfit trace

- Let $B(\mathbf{m})=F(\mathbf{m})-D \in \mathbb{R}^{1 \times s}$. In $k$ th iteration, $\mathbf{m}=\mathbf{m}_{k}$.
- Then $A=B^{T} B$ is implicit symmetric positive semi-definite (SPSD); effectively, can only carry out matrix-vector products $A * \mathbf{v}$ with this $s \times s$ matrix.

$$
\phi(\mathbf{m})=\|B(\mathbf{m})\|_{F}^{2}=\operatorname{tr}\left(B^{T} B\right)=\mathbb{E}\left(\mathbf{w}^{T} A \mathbf{w}\right) .
$$

- Approximating expectation $\Leftrightarrow$ Approximating the trace $\phi(\mathbf{m})=\operatorname{tr}(A)$
- Monte-Carlo approximation

$$
\operatorname{tr}(A) \approx \frac{1}{s_{k}} \sum_{j=1}^{s_{k}} \mathbf{w}_{j}^{T} A \mathbf{w}_{j}=\frac{1}{s_{k}} \sum_{j=1}^{s_{k}}\left\|B \mathbf{w}_{j}\right\|_{2}^{2} .
$$

- Note we can obtain exact trace using $s_{k}=s$ samples with $\mathbf{w}_{j}$ a scaled $j$ th column of identity; but we want $s_{k} \ll s$.


## Using stabilized Gauss-Newton with total VARIATION (TV) ADDED

| Method | Vanilla $(3,969)$ | Gaussian $(3,969)$ | Vanilla (49) |
| :--- | :---: | :---: | :---: |
| Work | 476,280 | 4,618 | 5,978 |


(g) True model

(h) Gaussian, $s=3,969$

(i) Vanilla, $s=49$

BUT what if $P=P_{i}$ varies with $i$, i.e., data for different experiments is not given at same locations?

## Using stabilized Gauss-Newton with total variation (TV) added

| Method | Vanilla $(3,969)$ | Gaussian $(3,969)$ | Vanilla (49) |
| :--- | :---: | :---: | :---: |
| Work | 476,280 | 4,618 | 5,978 |


(j) True model

(k) Gaussian, $s=3,969$

(I) Vanilla, $\mathrm{s}=49$

BUT what if $P=P_{i}$ varies with $i$, i.e., data for different experiments is not given at same locations?
Can no longer write $\sum_{i=1}^{s} w_{i} P G(\mathbf{m}) \mathbf{q}_{i}=\sum_{i=1}^{s} P G(\mathbf{m})\left(w_{i} \mathbf{q}_{i}\right)$, and the magic of the randomized algorithm is gone.

## DATA APPROXIMATION METHODS

Let receivers of $i$ th data set be in $\Gamma_{i} \subset \partial \Omega, i=1,2, \ldots, s$. Want to extend data to the union $\Gamma=\bigcup \Gamma_{i} \subseteq \partial \Omega$.
(1) DCT, wavelets, curvelets for each $i$. Advantage: leverage the recent advances in compressive sensing and sparse $\ell_{1}$ methods.
(2) Piecewise linear interpolation for each $v_{i}$. Advantage: very simple.
(3) L2G: data completion function $v_{i} \in H^{1}(\Gamma)$ solves discretization of

$$
\min _{v}\left\|v-\mathbf{d}_{i}\right\|_{L_{2}\left(\Gamma_{i}\right)}^{2}+\beta\left\|\nabla_{S} v\right\|_{L_{2}(\Gamma)}^{2} .
$$

(9) Data completion function $v_{i} \in H^{2}(\Gamma)$ solves discretization of

$$
\min _{v}\left\|v-\mathbf{d}_{i}\right\|_{L_{2}\left(\Gamma_{i}\right)}^{2}+\beta\left\|\Delta_{S} v\right\|_{L_{2}(\Gamma)}^{2} .
$$

Which method to use?

## Choosing data Approximation method

- Use Mathematics, not Politics, to select method: this approach can work in practice.
- Concentrate on EIT / DC resistivity with piecewise smooth conductivity $\mu(\mathbf{x})$.
(1) If $\mu$ 's discontinuities are all away from boundary, then $u \in H^{2}(\Gamma)$. So, use regularization with Laplacian (Option 4).
(2) If $\mu$ has discontinuities which extend to boundary, then $u \in H^{1}(\Gamma)$. So, use L2G (Option 3).

See [ Roosta, Doel \& A., 2014] for theorems justifying the above.

## Choosing data approximation method

Experiments with 50\% data completion and 5\% noise:


Left: Laplacian for $u \in H^{2}(\Gamma)$. Right: L2G for $u \in H^{1}(\Gamma)$

## $\mu_{I}=.1, \mu_{I I}=1$, NoISE $3 \%, s=961$, COMP. $20 \%$

Compare using Gaussian distribution with data completion vs random subset which does not require data completion.

| Method | Random Subset | Data Completion |
| :--- | :---: | :---: |
| Work | 3,367 | 1,597 |



Left: true. Center: RS. Right: DC

## $\mu_{I}=.1, \mu_{I I}=1$, NOISE $3 \%, s=961$, COMP. $20 \%$

Compare using Gaussian distribution with data completion vs random subset which does not require data completion.

| Method | Random Subset | Data Completion |
| :--- | :---: | :---: |
| Work | 6,302 | 2,769 |



Left: true. Center: RS. Right: DC

## $\mu_{I}=1, \mu_{I I}=.1$, NOISE $5 \%, s=961$, COMP. $50 \%$

Compare using Gaussian distribution with data completion vs random subset which does not require data completion.

| Method | Random Subset | Data Completion |
| :--- | :---: | :---: |
| Work | 5,139 | 2,320 |



Left: true. Center: RS. Right: DC

## $\mu_{I}=1, \mu_{I I}=.1$, NOISE $5 \%, s=961$, COMP. $50 \%$

Compare using Gaussian distribution with data completion vs random subset which does not require data completion.

| Method | Random Subset | Data Completion |
| :--- | :---: | :---: |
| Work | 5,025 | 1,818 |



Left: true. Center: RS. Right: DC

## Summary and moreover

- In the accompanying paper there are also 3D results, similar to the ones for the case with the same receivers.
- Both variants with and without level set method were tried.
- The Data Completion method was always faster than Random Subset by a factor of at least 2 and up to 4 .
- Data completion of up to $\approx 50 \%$ works fine. But reconstructions deteriorate upon completing scarcer data!


## Outline

- Motivation
- Completing scarce (sparse) data
- Uncertainty in data locations
- Forced to cut corners?
- Randomized algorithms for many data sets
- Conclusions


## Conclusions

- Data completion and other statistically unholy manipulations such as ignoring location uncertainty are not an ideal undertaking from a theoretical point of view.
- But in practical situations it is often quietly done by mathematicians, computer scientists and engineers alike.
- We have seen instances where (more massive) such practices should be avoided.
- We have seen instances where such practices can be tolerated, typically when other uncertainties dominate.
- We have seen instances where such practices seem essential for obtaining plausible results, and where better algorithms are further sought.
- The larger the proportion of missing data, the harder it is to produce an adequate completed set.


## Conclusions Conclusions

## BAYES MADE ME DO IT

## When All Else Fails <br> manipulate the data

