Iterative Projection and Reflection Methods

Theory and Applications

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PhD Completion Seminar
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Statement of Research

My thesis is concerned with the, so called, feasibility problem which asks:

$$\text{find } x \in C := \bigcap_{j=1}^{N} C_j \subseteq \mathcal{H},$$

where $C_1, C_2, \ldots, C_N$ are closed subsets of a Hilbert space $\mathcal{H}$.

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Within this framework, my thesis is concerned with:

- theory and algorithms,
- mathematical modelling and applications.

Contributions are made to each of these areas.

Of particular interest are iterative algorithms which used nearest point projectors and their corresponding reflectors.

Main Findings to Date: Summary

Theory and algorithms:

- ⋆ Developed the cyclic Douglas–Rachford algorithm and variants.
  - For convex sets, proved convergence to solutions (if they exist),
  - Characterised behaviour if no solutions exists.
- Proof of norm convergence for moment problems.
- Theoretical foundation to explain existing ptychographic imaging algorithms in the imaging community.
- Global convergence for structured non-convex problems without local regularity.

Modelling and Applications:

- Case studies on combinatorial optimisation problems.
- Systematic treatment of matrix completion problems.
  - ⋆ Distance matrix reconstruction arising in protein folding.
  - ⋆ Ongoing work is concerned with using regularity notions of collections of sets to prove local convergence (some partial results).

Algorithmic Building Blocks

Let $S \subseteq \mathcal{H}$ be non-empty. The (nearest point) projection onto S is the (set-valued) mapping,

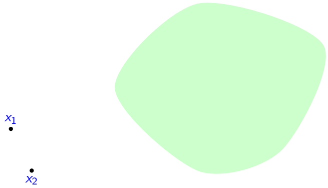
$$P_S x := \left\{ s \in S : \|x - s\| \leq \inf_{s \in S} \|x - s\| \right\}.$$

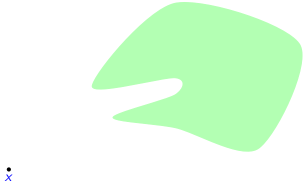
If S is closed and convex then projections exists uniquely with

$$P_S(x) = p \iff \langle x - p, s - p \rangle \leq 0 \text{ for all } s \in S.$$

The reflection w.r.t. S is the (set-valued) mapping,

$$R_S := 2P_S - I.$$





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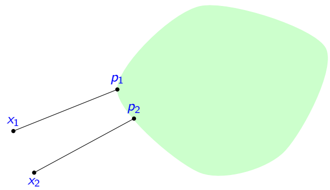

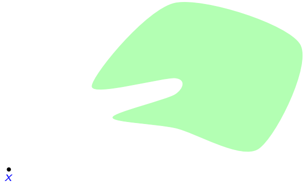

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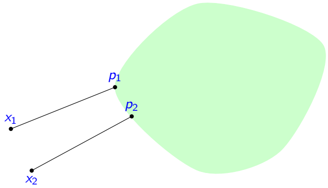

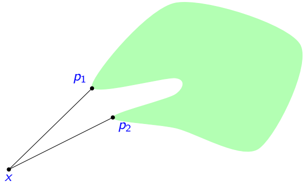

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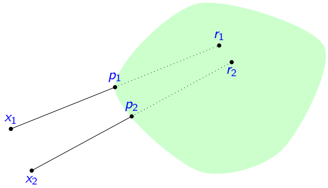

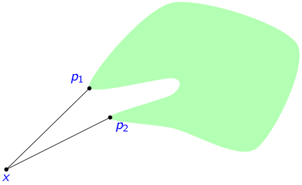

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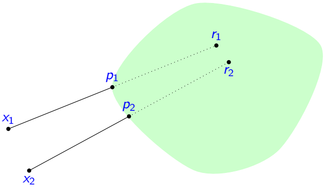
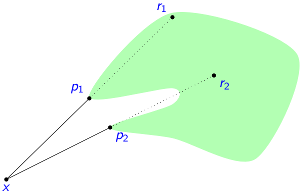




The Douglas–Rachford Operator and Algorithm

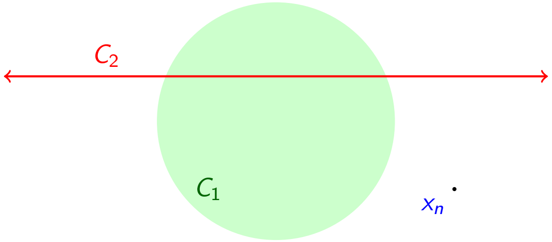
Given an initial point $x_0 \in \mathcal{H}$, the Douglas–Rachford method is the fixed-point iteration given by

$$x_{n+1} \in T_{C_1,C_2} x_n \quad \text{where} \quad T_{C_1,C_2} := \frac{Id + R_{C_2} R_{C_1}}{2}.$$

Theorem (Douglas–Rachford–Peaceman, Lions–Mercier,...)

Let $C_1, C_2 \subseteq \mathcal{H}$ be closed and convex with $C_1 \cap C_2 \neq \emptyset$ then $x_n \overset{w.}{\rightharpoonup} x$ s.t. $P_{C_1}(x) \in C_1 \cap C_2$.

- More generally, if $x \in \text{Fix}\, T_{1,2}$ there exists an element of $P_{C_1} x$ contained in in the intersection.



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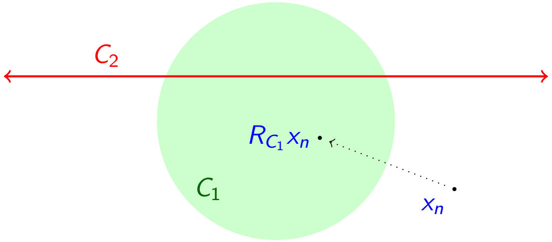

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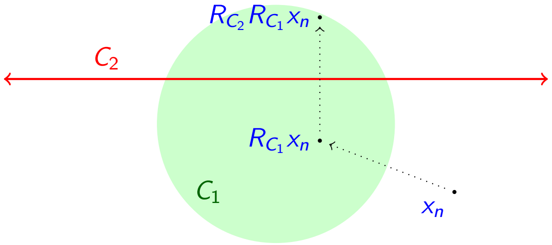

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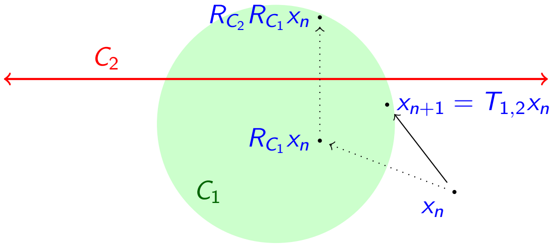

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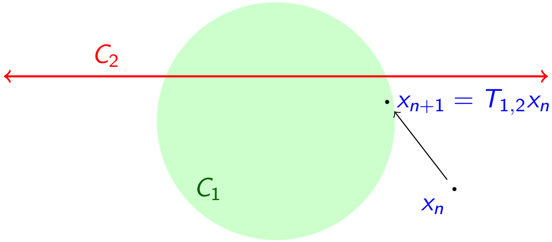

Pierra's Product Space Reformulation

For our constraint sets $C_1, C_2, \dots, C_N \subseteq \mathcal{H}$ we define

$$\mathbf{D} := \{(x, x, \dots, x) \in \mathcal{H}^N : x \in \mathcal{H}\}, \quad \mathbf{C} := \prod_{j=1}^{N} C_j.$$

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We now have an equivalent two set feasibility problem (in $\mathcal{H}^N$) as

$$x \in \bigcap_{j=1}^{N} C_j \subseteq \mathcal{H} \iff (x, x, \ldots, x) \in \mathbf{D} \cap \mathbf{C} \subseteq \mathcal{H}^N.$$

Moreover the projections onto the new sets can be computed whenever $P_{C_1}, P_{C_2}, \ldots, P_{C_N}$. Denote $\mathbf{x} = (x_1, x_2, \ldots, x_N)$ they are given by

$$P_{\mathbf{D}}(\mathbf{x}) = \left(\frac{1}{N}\sum_{j=1}^{N} x_i\right)_{j=1}^{N} \quad \text{and} \quad P_{\mathbf{C}}(\mathbf{x}) = \prod_{j=1}^{N} P_{C_j} x_j.$$

Cyclic Douglas–Rachford Method

Theorem (Borwein–T 2013)

Let $C_1, C_2, \ldots, C_N \subseteq \mathcal{H}$ be closed and convex with non-empty intersection. Given $x_0 \in \mathcal{H}$ define

$$x_{n+1} := \underbrace{\left(T_{C_N,C_1} T_{C_{N-1},C_N} \ldots T_{C_2,C_3} T_{C_1,C_2}\right)}_{=: T_{[1\,2\,\ldots\,N]}} x_n \text{ where } T_{C_j,C_{j+1}} = \frac{I + R_{C_{j+1}} R_{C_j}}{2}.$$

Then (x_n) converges weakly to a point x such that $P_{C_1}x = \cdots = P_{C_N}x$.

- Using Hundal (2004): There exists a hyperplane and convex cone with nonempty intersection such that convergence is not strong.
- Bauschke–Noll–Phan (2014): If $\dim \mathcal{H} < \infty$ and $\cap_{j=1}^N \operatorname{ri} C_j \neq \emptyset$ then convergence is linear.
- Bauschke–Noll–Phan (2014): If $\operatorname{Fix} T_{[1\,2\,\ldots\,N]}$ is boundedly linearly regular and $C_j + C_{j+1}$ is closed, for each j, then convergence is linear.
- **Borwein–T (2015):** Characterised behaviour for empty intersections.

Cyclic Douglas–Rachford Method

The difficulty in extending to (potentially) non-empty intersections, is that $\text{Fix } T_{C_i,C_{i+1}} \neq \emptyset \iff C_i \cap C_{i+1} \neq \emptyset$, and the proof uses:

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To proceed is necessary to consider the "atoms" of the operator $T_{[C_1\, C_2 \dots\, C_N]}$ more directly:

$$\boxed{\dots \mapsto \quad x_n \overset{T_{[C_1\, C_2 \dots\, C_N]}}{\mapsto} x_{n+1} \mapsto \dots}$$

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$$\Downarrow$$

$$\boxed{\dots \mapsto x_n^1 \overset{T_{C_1,C_2}}{\mapsto} x_n^2 \overset{T_{C_2,C_3}}{\mapsto} \dots \overset{T_{C_{N-1},C_N}}{\mapsto} x_n^N \overset{T_{C_N,C_1}}{\mapsto} x_{n+1}^1 \mapsto \dots} \qquad (*)$$

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Denoting $T_{[\sigma_1]} := T_{[C_1\, C_2 \dots C_N]}$, $T_{[\sigma_2]} := T_{[C_2 \dots C_N\, C_1]}$, and so on. We were able to prove the following dichotomy theorem.

Theorem (Borwein–T 2015)

Let $C_1, C_2, \dots, C_N \subseteq \mathcal{H}$ be closed and convex. Then:

(a) For all $i \in \{1, 2, \dots, N\}$,

$$P_{C_{i+1}} R_{C_i} x_n^i - P_{C_{i+1}} x_n^i = (x_n^{i+1} - x_n^i) - (P_{C_{i+1}} x_n^{i+1} - P_{C_i} x_n^i) \to 0.$$

(b) Exactly one of the following alternatives hold.

  (i) Each Fix $T_{[\sigma_i]}$ is empty. Then $\|x_n^i\| \to +\infty$.

  (ii) Each Fix $T_{[\sigma_i]}$ is nonempty. Then, for each i,

$$x_n^i \overset{w}{\rightharpoonup} x^i \in \text{Fix } T_{[\sigma_i]} \text{ with } x^{i+1} = T_{i,i+1} x^i.$$

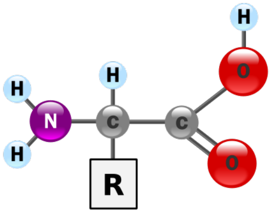
  Furthermore, there exists $d^1, \dots, d^N \in \mathcal{H}$ dependent only on the constraint sets such that

$$x_n^{i+1} - x_n^i = P_{C_{i+1}} R_{C_i} x_n^i - P_{C_i} x_n^i \to d^i, \quad P_{C_{i+1}} x_n^{i+1} - P_{C_i} x_n^i \to d^i,$$

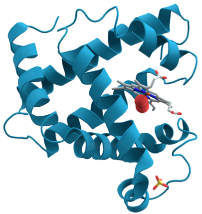
$$x^{i+1} - x^i = P_{C_{i+1}} x^{i+1} - P_{C_i} x^i = d^i, \qquad P_{C_{i+1}} R_{C_i} x^i = P_{C_{i+1}} x^{i+1}.$$

Protein Conformation Determination and EDMs

Proteins are large biomolecules comprising of multiple amino acid chains.



Generic amino acid



Myoglobin

They participate in virtually every cellular process, and knowledge of structural conformation gives insights into the mechanisms by which they perform.

Protein Conformation Determination and EDMs

One technique that can be used to determine conformation is nuclear magnetic resonance (NMR) spectroscopy. However, NMR is only able to resolve short inter-atomic distances (*i.e.*, < 6Å). For 1PTQ (404 atoms) this corresponds to $< 8\%$ of the total inter-atomic distances.

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We say $D = (D_{ij}) \in \mathbb{R}^{m\times m}$ is a Euclidean distance matrix (EDM) if there exists points $p_1, \dots, p_m \in \mathbb{R}^q$ such that

$$D_{ij} = \|p_i - p_j\|^2.$$

When this holds for points in $\mathbb{R}^q$, we say that D is embeddable in $\mathbb{R}^q$.

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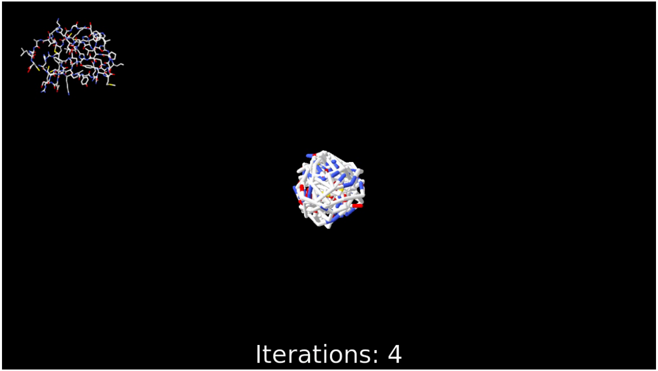
We formulate protein reconstruction as a matrix completion problem:

Find a EDM, embeddable in $\mathbb{R}^s$ where $s := 3$,
knowing only short inter-atomic distances.

The Algorithm in Action: 1PTQ

The following animation shows the reconstruction of 1PTQ. The EDM reconstruction problem has 81,000 entries of which only 9% are known.



First 3,000 steps of the 1PTQ reconstruction

http://carma.newcastle.edu.au/DRmethods/1PTQ.html

A Feasibility Problem Formulation

Denote by Q the Householder matrix defined by

$$Q := I - \frac{2vv^T}{v^Tv}, \text{where } v = \left[1, 1, \ldots, 1, 1 + \sqrt{m}\right]^T \in \mathbb{R}^m.$$

Theorem (Hayden–Wells 1988)

A nonnegative, symmetric, hollow matrix X, is a EDM iff $\widehat{X} \in \mathbb{R}^{(m-1)\times(m-1)}$ in

$$Q(-X)Q = \begin{bmatrix} \widehat{X} & d \\ d^T & \delta \end{bmatrix} \qquad (*)$$

is positive semi-definite (PSD). In this case, X is embeddable in $\mathbb{R}^q$ where $q = \operatorname{rank}(\widehat{X}) \leq m-1$ but not in $\mathbb{R}^{q-1}$.

Let D denote the partial EDM (obtained from NMR), and $\Omega \subset \mathbb{N} \times \mathbb{N}$ the set of indices for known entries. The problem of low-dimensional EDM reconstruction can thus be case as a feasibility problem with constraints:

$$C_1 = \{X \in \mathbb{S}^{m\times m} : X \geq 0, X_{ij} = D_{ij} \text{ for } (i,j) \in \Omega\},$$
$$C_2 = \{X \in \mathbb{S}^{m\times m} : \widehat{X} \text{ in } (*) \text{ is PSD with } \operatorname{rank} \widehat{X} \leq s := 3\}.$$

Computing Projections and Reflections

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The projection onto C_1 is given (point-wise) by

$$P_{C_1}(X)_{ij} = \begin{cases} D_{ij} & \text{if } (i,j) \in \Omega, \\ \max\{0, X_{ij}\} & \text{otherwise.} \end{cases}$$

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Recall the constraint sets:

$$C_1 = \{X \in \mathbb{S}^{m\times m} : X \geq 0, X_{ij} = D_{ij} \text{ for } (i,j) \in \Omega\},$$
$$C_2 = \{X \in \mathbb{S}^{m\times m} : \widehat{X} \text{ in } (*) \text{ is PSD with } \operatorname{rank} \widehat{X} \leq s := 3\}.$$

The projection onto C_1 is given (point-wise) by

$$P_{C_1}(X)_{ij} = \begin{cases} D_{ij} & \text{if } (i,j) \in \Omega, \\ \max\{0, X_{ij}\} & \text{otherwise.} \end{cases}$$

The projection onto C_2 is the set

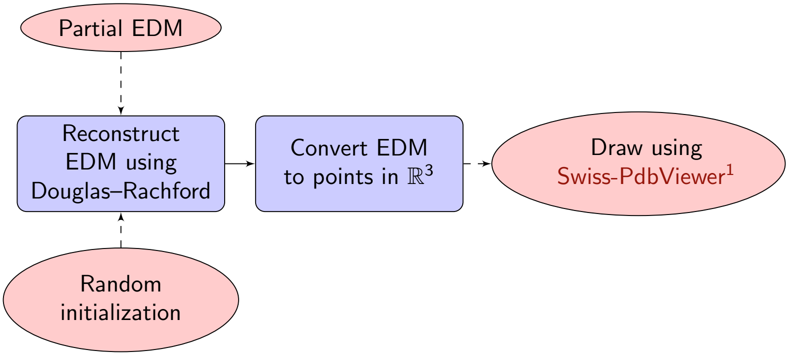
$$P_{C_2}(X) = \left\{ -Q \begin{bmatrix} \widehat{Y} & d \\ d^T & \delta \end{bmatrix} Q : Q(-X)Q = \begin{bmatrix} \widehat{X} & d \\ d^T & \delta \end{bmatrix}, \begin{array}{l} \widehat{X} \in \mathbb{R}^{(m-1)\times(m-1)}, \\ d \in \mathbb{R}^{m-1}, \delta \in \mathbb{R}, \end{array} \widehat{Y} \in P_{\mathcal{S}_3}\widehat{X} \right\},$$

where $\mathcal{S}_s$ is the set of PSD matrices of rank s or less.

- Computing $P_{\mathcal{S}_s}(\widehat{X}) =$ spectral decomposition $\rightarrow$ threshold eigenvalues.

The Algorithmic Approach

The reconstruction approach can be summarised as follows:



[1] http://spdbv.vital-it.ch/

Strategies for Proving Convergence

Given $\overline{X} \in C_1 \cap C_2$, in order to guarantee local convergence the current *state-of-the-art* requires two local properties:

1. strong regularity of the intersection at $\overline{X}$:
$$N_{C_1}(\overline{X}) \cap \left(-N_{C_2}(\overline{X})\right) = \{0\}.$$
2. superregularity of both C_1 and C_2 at $\overline{X}$: $(j = 1, 2)(\forall \epsilon > 0)(\exists \delta > 0)$
$$\langle V, \overline{X} - X \rangle \leq \epsilon \|V\| \|\overline{X} - X\|,$$
for all $V \in N_{C_j}(\overline{X})$, $X \in \mathbb{B}_\delta(\overline{X}) \cap C_j$.

[1] Here $N_\Omega(\overline{x})$ denotes the Mordukhovich (limiting) normal cone:
$$N_\Omega(\overline{x}) := \{y : \exists (x_n), (y_n) \text{ s.t. } x_n \to \overline{x},\ y_n \to y,\ y_n \in \mathbb{R}_+(x_n - P_\Omega(x_n))\}.$$

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With some work, for EDM reconstruction, we have shown these sufficient conditions to be equivalent to the existence of a non-zero solution to a certain linear system defined by the experimental data:

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$$(Y, \widehat{Y}) \in \mathbb{S}^{m+1} \times \mathbb{S}^m \text{ s.t. } Q(-Y)Q = \begin{bmatrix} \widehat{Y} & 0 \\ 0 & 0 \end{bmatrix}, \widehat{X}\widehat{Y} = 0, Y_{ij} = 0 \text{ for all } (i,j) \notin \Omega.$$

- A checkable sufficient condition for local convergence!

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A stronger property prox-regularity implies supperregularity.

- For realistic solutions, we have shown the former always holds.
- Yields no quantitative relationship between ϵ and δ.
- Needed in order to say something about the convergence rate!

Research Timeline & Obstacles to Completion

Ongoing projects and writing:

- ✓ ~~July 2015: Complete global convergence of structured non-convex Douglas–Rachford iterations investigation.~~
- September 2015: Complete local convergence investigation for EDM reconstruction.
- November 2015: Complete first draft of thesis.
- December 2015: Submit thesis.

Conference Participation and Academic Visits:

- August 2015: Heidelberg Laureate Forum (1 week).
- September 2015: Visit Prof Luke at Uni. Göttingen (1 week).
- October 2015: Present at the Annual AustMS meeting.
- December 2015: Apply for AustMS Lift-Off Fellowship.

I declare no obstacles to completion.

References and Publications

Theory and Algorithms:

A cyclic Douglas–Rachford iteration scheme.
J.M. Borwein & M.K. Tam. *JOTA*, 160(1):1–29, 2014.

The cyclic Douglas–Rachford method for inconsistent feasibility problems.
J.M. Borwein & M.K. Tam. *J. Nonlinear Convex Anal.*, 16(4):537–584, 2015.

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F.J. Aragón Artacho, J.M. Borwein & M.K. Tam. *Submitted to J. Glob. Optim.*

Modelling and Applications:

Reflection methods for inverse problems with applications to protein conformation determination. J.M. Borwein and M.K. Tam, *Generalized Nash Equilibrium Problems, Bilevel Prog. and MPEC.* In Press, Springer (2014).

Douglas–Rachford feasibility methods for matrix completion problems.
F.J. Aragón Artacho, J.M. Borwein & M.K. Tam. *ANZIAM J.* 55(4):299–326 (2014)

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