Inverse Problems in Imaging
Lecture 4

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UCL, Term 2

Outline

1. Iterative Methods
   - Gradient Descent and Landweber Method
   - Conjugate Gradients
   - Regularisation within Iterative Methods
   - LSQR

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- This leads to the requirement for iterative methods.
- We first consider linear problems.

Consider the minimisation of a quadratic form

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The gradient is

$$\nabla_{\boldsymbol{f}}\Phi(\boldsymbol{f}, \boldsymbol{g}) = \mathrm{A}^{\mathrm{T}}\mathrm{A}\boldsymbol{f} - \mathrm{A}^{\mathrm{T}}\boldsymbol{g} \qquad (4.2)$$

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Given an approximation $\boldsymbol{f}_k$ for the solutions, in a neighbourhood of the point the functional Φ decreases most rapidly in the direction of the *negative* gradient, i.e. in the direction of the residual $\boldsymbol{r}$. Thus for small values τ, we can guarantee that a new solution

$$\boldsymbol{f}_{k+1} = \boldsymbol{f}_k + \tau\boldsymbol{r}_k \tag{4.4}$$

will give a smaller value of Φ.

How do we choose τ ?

[1] More generally the minimisation of the one-dimensional functional $\phi(\tau)$ would be non-quadratic and would require a *line-search* method.

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$$\phi(\tau) = \Phi(\boldsymbol{f}_k + \tau \boldsymbol{r}_k, \boldsymbol{g}) = \Phi(\boldsymbol{f}_k, \boldsymbol{g}) + \frac{\tau^2}{2} ||\mathsf{A}\boldsymbol{r}_k||^2 - \tau ||\boldsymbol{r}_k||^2 \,. \tag{4.5}$$

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Since this is a quadratic function of τ we have immediately that

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- They satisfy an orthogonality condition

$$\langle \boldsymbol{r}_{k+1}, \boldsymbol{r}_k \rangle = 0 \,. \tag{4.8}$$

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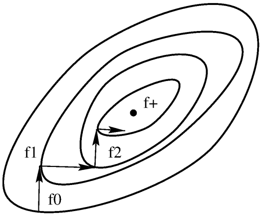

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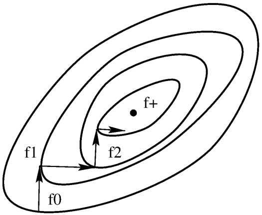

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Iterative Methods

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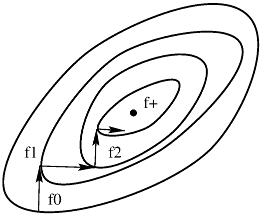

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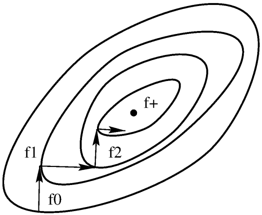

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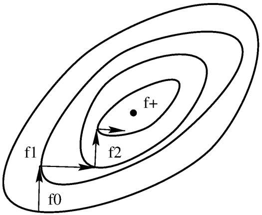

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- Stopping the iterations before minimisation has a regularising effect.
- It can be unreasonably slow : In the case of an anisotropic optimisation surface, the iterations can only descend very gradually to the minimum.
- It is almost always better to use a conjugate gradient method!

Two vectors $\boldsymbol{p}$ and $\boldsymbol{q}$ are said to be conjugate with respect to a matrix B if

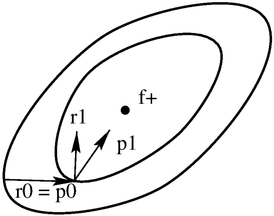
$$\langle \boldsymbol{p}, \mathrm{B}\boldsymbol{q} \rangle = 0$$

Then, given any level surface (ellipsoid) of the discrepency functional and a point on this surface, the direction of the conjugate gradient at this point is the direction orthogonal to the tangent plane w.r.t the matrix $\mathrm{A}^{\mathrm{T}}\mathrm{A}$.
We observe that a descent method such as described in the previous section builds the solution at the j^{th} iteration, from a vector space spanned by the set of vectors

$$\mathcal{K}^{(j)}(\mathrm{A}, \boldsymbol{g}) = \left\{ \mathrm{A}^{\mathrm{T}}\boldsymbol{g}, \mathrm{A}^{\mathrm{T}}\mathrm{A}\mathrm{A}^{\mathrm{T}}\boldsymbol{g}, \ldots \left(\mathrm{A}^{\mathrm{T}}\mathrm{A}\right)^{(j)} \mathrm{A}^{\mathrm{T}}\boldsymbol{g} \right\} \tag{4.9}$$

where it is assumed that all of the vectors in the set are mutually independent. This space is called the *Krylov subspace* of A.

- An optimal solution may be found by choosing at each iteration a direction that is the least-squares solution in this Krylov subspace.
- At the first iteration the subspace is of dimension one, and our only choice is the same as steepest descents.
- At subsequent directions we choose a direction that points towards the centre of an ellipsoid given by the intersection of the functional level surface with the Krylov subspace.



If P_j is the projection operator onto $\mathcal{K}^{(j)}(\mathrm{A}, \boldsymbol{g})$ then we need to solve

$$\begin{aligned} ||\mathrm{A}\mathrm{P}_j \boldsymbol{f} - \boldsymbol{g}||^2 \quad &\rightarrow \quad \min \\ \text{subject to} \quad & \quad \mathrm{P}_j \boldsymbol{f} = \boldsymbol{f} \end{aligned} \tag{4.10}$$

which is given by

$$\mathrm{P}_j^{\mathrm{T}} \mathrm{A}^{\mathrm{T}} \mathrm{A} \mathrm{P}_j \boldsymbol{f} = \mathrm{P}_j \mathrm{A}^{\mathrm{T}} \boldsymbol{g} \tag{4.11}$$

The CG method is based on the construction of two bases $\{\boldsymbol{r}_k\}$ and $\{\boldsymbol{p}_k\}$ as follows

-
$$\boldsymbol{r}_0 = \boldsymbol{p}_0 = \mathrm{A}^{\mathrm{T}}\boldsymbol{g} \tag{4.12}$$

- compute
$$\alpha_k = \frac{||\boldsymbol{r}_k||^2}{\langle \boldsymbol{r}_k, \mathrm{A}^{\mathrm{T}}\mathrm{A}\boldsymbol{p}_k \rangle} \tag{4.13}$$

- compute
$$\boldsymbol{r}_{k+1} = \boldsymbol{r}_k - \alpha_k \mathrm{A}^{\mathrm{T}}\mathrm{A}\boldsymbol{p}_k \tag{4.14}$$

- compute
$$\beta_k = \frac{\langle \boldsymbol{r}_{k+1}, \mathrm{A}^{\mathrm{T}}\mathrm{A}\boldsymbol{p}_k \rangle}{\langle \boldsymbol{p}_k, \mathrm{A}^{\mathrm{T}}\mathrm{A}\boldsymbol{p}_k \rangle} \tag{4.15}$$

- compute
$$\boldsymbol{p}_{k+1} = \boldsymbol{r}_{k+1} + \beta_k \boldsymbol{p}_k \tag{4.16}$$

Then the iterative scheme for the solutions is

$$\begin{aligned} \boldsymbol{f}_0 &= 0 \\ \boldsymbol{f}_{k+1} &= \boldsymbol{f}_k + \alpha_k \boldsymbol{p}_k \end{aligned} \tag{4.17}$$

The coefficients α_k, β_k are chosen so that the following orthogonality conditions hold $\langle \boldsymbol{r}_{k+1}, \boldsymbol{r}_k \rangle = 0\,, \quad \langle \boldsymbol{p}_{k+1}, \mathrm{A}^{\mathrm{T}}\mathrm{A}\boldsymbol{p}_k \rangle = 0\,,$

i.e. the sequence of $\{\boldsymbol{r}_k\}$ are such that $\boldsymbol{r}_1 \perp \boldsymbol{r}_0$, $\boldsymbol{r}_2 \perp \boldsymbol{r}_1$, etc. and $\boldsymbol{p}_1$ is conjugate to $\boldsymbol{p}_0$, $\boldsymbol{p}_2$ is conjugate to $\boldsymbol{p}_1$ etc. Furthermore we can show that

- the set $\{\boldsymbol{r}_k, k = 0 \ldots j\}$ form an orthogonal basis of $\mathcal{K}^{(j)}(\mathrm{A}, \boldsymbol{g})$,
- the set $\{\boldsymbol{p}_k, k = 0 \ldots j\}$ form an $\mathrm{A}^{\mathrm{T}}\mathrm{A}$-orthogonal basis of $\mathcal{K}^{(j)}(\mathrm{A}, \boldsymbol{g})$,
- the set $\{\boldsymbol{r}_k, k = 0 \ldots j\}$ are the residuals

$$\boldsymbol{r}_k = \mathrm{A}^{\mathrm{T}}\boldsymbol{g} - \mathrm{A}^{\mathrm{T}}\mathrm{A}\boldsymbol{f}_k$$

Comment: the following alternative expression for α_k, β_k holds :

$$\alpha_k = \frac{||\boldsymbol{r}_k||^2}{\langle \boldsymbol{p}_k, \mathrm{A}^{\mathrm{T}}\mathrm{A}\boldsymbol{p}_k \rangle} \qquad \beta_k = \frac{||\boldsymbol{r}_{k+1}||^2}{||\boldsymbol{r}_k||^2}$$

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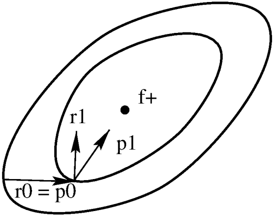

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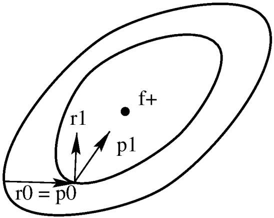

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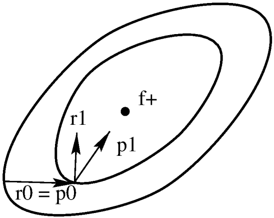
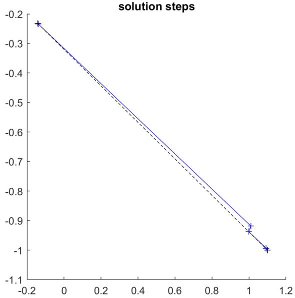
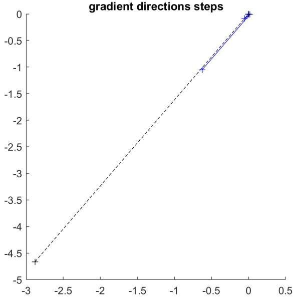
- If the problem is $n-$dimensional we reach the minimum in n steps.



Results from code : `RunGradToy`.



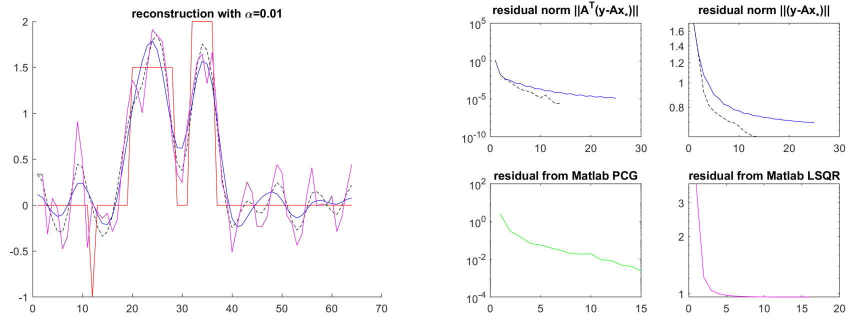


SD iterations

$$\begin{pmatrix} -0.1394 & 1.0103 & 0.9989 & 1.0927 & 1.0918 & 1.0994 & 1.0993 & 1.10 \\ -0.2341 & -0.9184 & -0.9375 & -0.9933 & -0.9949 & -0.9995 & -0.9996 & -1.00 \end{pmatrix}$$

CG iterations $\begin{pmatrix} -0.1432 & 1.1000 \\ -0.2317 & -1.0000 \end{pmatrix}$

Results from code : `RunGradLinBlur`.



Left: Results from solving normal equations $(A^TA + \alpha I)\boldsymbol{f} = A^T\boldsymbol{g}$ with SteepestDescent (blue) and CG (dashed black), and LSQR equations (magenta). Right : residual norms using Steepest Descent, CG, and Matlab functions `pcg` and `lsqr`.

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- if $\Gamma = \mathsf{I}$ then the generated Krylov space is just an affine transformation of eq. 4.9 and therefore the same space of solutions are reached **but a different norm is minimised**.

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- (One of the) differences between different Krylov solvers corresponds to the definition of what norm is being minimised

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- We have to supply the Matlab function `lsqr` with a "stacked" matrix and source vector e.g

$$\boldsymbol{f} = \mathtt{lsqr}\left(\begin{pmatrix} \mathrm{A} \\ \sqrt{\alpha}\mathrm{L} \end{pmatrix}, \begin{pmatrix} \boldsymbol{g} \\ \mathbf{0} \end{pmatrix}, \ldots \right)$$

Or the equivalent function handle. See documentation!