Quick Recap: — Global Convergence and Enhancements

We looked at some theorems describing the convergence of our algorithms. We noted that there was a bit of a gap between what is generally true/practical, and what can be proved. (Theoretical limit points vs. numerical stopping criteria.)

Further, we looked at some enhancements including scaling

\[ D = \text{diag}(d_1, d_2, \ldots, d_n), \quad d_i > 0, \quad T(\Delta) = \{ \bar{p} \in \mathbb{R}^n : \|D\bar{p}\| \leq \Delta \}, \]

and the use of non-Euclidean norms — the latter primarily come in handy in the context of constrained optimization.

We now explore an important computational tool, which will help us solve problems of realistic size. — Conjugate Gradient Methods.
Conjugate Directions

Definition (Conjugate Vector)
A set of nonzero vectors \( \{ \bar{p}_0, \bar{p}_1, \ldots, \bar{p}_{n-1} \} \) is said to be conjugate with respect to the symmetric positive definite matrix \( A \) if
\[
\bar{p}_i^T A \bar{p}_j = 0, \quad \forall i \neq j.
\]

Property: Linear Independence of Conjugate Vectors
A set of conjugate vectors \( \{ \bar{p}_0, \bar{p}_1, \ldots, \bar{p}_{n-1} \} \) is linearly independent.

Why should we care? — We can minimize \( \Phi(\bar{x}) \) in \( n \) steps by successively minimizing along the directions in a conjugate set...

Conjugate Direction Method (\( \neq \) CG Method)

The linear CG method is an iterative method for solving linear systems of equations:
\[
A\bar{x} = \bar{b}, \quad A \in \mathbb{R}^{n \times n}, \quad \bar{x} \in \mathbb{R}^n, \quad \bar{b} \in \mathbb{R}^n,
\]
where the matrix \( A \) is symmetric positive definite.

Notice/Recall: This problem is equivalent to minimizing \( \Phi(\bar{x}) \) where
\[
\Phi(\bar{x}) = \frac{1}{2} \bar{x}^T A \bar{x} - \bar{b}^T \bar{x} + c,
\]
since
\[
\nabla \Phi(\bar{x}) = A\bar{x} - \bar{b} \quad \text{def} \quad = \bar{r}(\bar{x}).
\]

We refer to \( \bar{r}(\bar{x}) \) as the residual of the linear system. Note that if \( \bar{x}^* = A^{-1} \bar{b} \), then \( \bar{r}(\bar{x}^*) = 0 \), i.e. the residual is a measure of how close (or far) we are from solving the linear system.

Given a starting point \( \bar{x}_0 \in \mathbb{R}^n \), and a set of conjugate directions \( \{ \bar{p}_0, \bar{p}_1, \ldots, \bar{p}_{n-1} \} \) we generate a sequence of points \( \bar{x}_k \in \mathbb{R}^n \) by setting
\[
\bar{x}_{k+1} = \bar{x}_k + \alpha_k \bar{p}_k,
\]
where \( \alpha_k \) is the minimizer of the quadratic function
\[
\varphi(\alpha) = \Phi(\bar{x}_k + \alpha \bar{p}_k), \quad \text{i.e. the minimizer of } \Phi(\cdot) \text{ along the line } \bar{r}(\alpha) = \bar{x}_k + \alpha \bar{p}_k.
\]
We have already solved this problem — in the context of step-length selection for line search methods, see lecture #6 — so we “know” that the optimizer is given by
\[
\alpha_k = -\frac{\bar{r}_k^T \bar{p}_k}{\bar{p}_k^T A \bar{p}_k}, \quad \text{where } \bar{r}_k = \bar{r}(\bar{x}_k).
\]

Theorem (\( n \)-step convergence)
For any \( \bar{x}_0 \in \mathbb{R}^n \) the sequence \( \{ \bar{x}_k \} \) generated by the conjugate direction algorithm converges to the solution \( \bar{x}^* \) of the linear system in at most \( n \) steps.

The proof indicates how properties of CG are found...

Since the directions \( \{ \bar{p}_i \} \) are linearly independent, they must span the whole space \( \mathbb{R}^n \). Hence, we can write
\[
\bar{x}^* - \bar{x}_0 = \sum_{k=0}^{n-1} \sigma_k \bar{p}_k
\]
for some choice of scalars \( \sigma_k \). We need to establish that \( \sigma_k = \alpha_k \). \( \square \)
Conjugate Direction Method  ( != CG Method )  3 of 4

Proof: Part 2.
If we are generating $\bar{x}_k$ by the conjugate direction method, then we have

$$\bar{x}_k = \bar{x}_0 + \alpha_0 \bar{p}_0 + \alpha_1 \bar{p}_1 + \cdots + \alpha_{k-1} \bar{p}_{k-1},$$

we multiply this by $\bar{p}_k^T A$

$$\bar{p}_k^T A \bar{x}_k = \bar{p}_k^T A [\bar{x}_0 + \alpha_0 \bar{p}_0 + \alpha_1 \bar{p}_1 + \cdots + \alpha_{k-1} \bar{p}_{k-1}],$$

using the conjugacy property, we see that all but the first term on the right-hand-side are zero:

$$\bar{p}_k^T A \bar{x}_k = \bar{p}_k^T A \bar{x}_0 \iff \bar{p}_k^T A (\bar{x}_k - \bar{x}_0) = 0.$$

Now we have

$$\bar{p}_k^T A (\bar{x}^* - \bar{x}_0) = \bar{p}_k^T A (\bar{x}^* - \bar{x}_0) = \bar{p}_k^T (\bar{b} - A \bar{x}_k) = -\bar{p}_k^T \bar{r}_k.$$  

Conjugate Direction Method: Comments and Interpretation  1 of 2

Most of the proofs regarding CD and CG methods are argued in a similar way — by looking at optimizers and residuals over sub-spaces of $\mathbb{R}^n$ spanned by some subset of a set of conjugate vectors.

**Interpretation:** If the matrix $A$ is diagonal, then the contours of $\Phi(\bar{x})$ are ellipses whose axes are aligned with the coordinate directions. In this case, we can find the minimizer by performing 1D-minimizations along the coordinate directions $\bar{e}_1, \bar{e}_2, \ldots, \bar{e}_n$ in turn.

Conjugate Direction Method  ( != CG Method )  4 of 4

Proof: Part 3.
We have shown

$$\bar{p}_k^T A (\bar{x}^* - \bar{x}_0) = -\bar{p}_k^T \bar{r}_k.$$

Now, we notice that the right-hand-side is the numerator in $\alpha_k$:

$$\alpha_k = -\bar{p}_k^T \bar{r}_k \implies \alpha_k = \frac{\bar{p}_k^T A (\bar{x}^* - \bar{x}_0)}{\bar{p}_k^T \bar{r}_k}.$$

We conclude the proof by showing that $\sigma_k$ can be expressed in the same manner; we premultiply the expression for $(\bar{x}^* - \bar{x}_0)$ by $\bar{p}_k^T A$ and obtain

$$\bar{p}_k^T A (\bar{x}^* - \bar{x}_0) = \bar{p}_k^T A \sum_{i=0}^{n-1} \sigma_i \bar{p}_i = \sum_{i=0}^{n-1} \sigma_i \bar{p}_k^T A \bar{p}_i = \sigma_k \bar{p}_k^T A \bar{p}_k.$$

Hence,

$$\sigma_k = \frac{\bar{p}_k^T A (\bar{x}^* - \bar{x}_0)}{\bar{p}_k^T \bar{r}_k} \equiv \alpha_k.$$

Conjugate Direction Method: Comments and Interpretation  2 of 2

**Interpretation (ctd.):** When $A$ is not diagonal, the contours are still elliptical, but are no longer aligned with the coordinate axes. Successive minimization along the coordinate directions $\bar{e}_1, \bar{e}_2, \ldots, \bar{e}_n$ can not guarantee convergence in $n$ (or even a (fixed) finite number of) iterations.
Recovering \( n \)-step Convergence for Non-Diagonal \( A \)

For non-diagonal matrices \( A \), the \( n \)-step convergence can be recovered by transforming the problem.

Let \( S \in \mathbb{R}^{n \times n} \) be a matrix with conjugate columns, \( i.e. \) if \( \{ \tilde{p}_0, \tilde{p}_1, \ldots, \tilde{p}_{n-1} \} \) is a set of conjugate directions (with respect to \( A \)), then

\[
S = \begin{bmatrix} \tilde{p}_0 & \tilde{p}_1 & \cdots & \tilde{p}_{n-1} \end{bmatrix}.
\]

We introduce a new variable \( \hat{x} = S^{-1}x \), and thus get the new quadratic objective which can be minimized in \( n \) steps

\[
\hat{\Phi}(\hat{x}) = \Phi(S\hat{x}) = \frac{1}{2} \hat{x}^T (S^T AS) \hat{x} - (S^T \tilde{b})^T \hat{x}.
\]

We note that the matrix \( (S^T AS) \) is diagonal by the conjugacy property, and that each coordinate direction \( \hat{e}_i \) in \( \hat{x} \)-space corresponds to the direction \( \tilde{p}_{i-1} \) in \( x \)-space.

When the matrix is diagonal, each coordinate minimization determines one of the components of the solution \( \tilde{x}^* \). Hence, after \( k \) iterations, the quadratic has been minimized on the subspace spanned by \( \tilde{e}_1, \tilde{e}_2, \ldots, \tilde{e}_k \).

If instead we minimize along the conjugate directions, then after \( k \) iterations, the quadratic has been minimized on the subspace spanned by \( \tilde{p}_0, \tilde{p}_1, \ldots, \tilde{p}_{k-1} \).

Expanding Subspace Minimization

Theorem (Expanding Subspace Minimization)

Let \( \tilde{x}_0 \in \mathbb{R}^n \) be any starting point and suppose that the sequence \( \{ \tilde{x}_k \} \) is generated by

\[
\tilde{x}_{k+1} = \tilde{x}_k + \alpha_k \tilde{p}_k,
\]

where \( \alpha_k = \frac{-\tilde{r}_k^T \tilde{p}_k}{\tilde{p}_k^T \tilde{A} \tilde{p}_k} \),

with \( \tilde{r}_k = A\tilde{x}_k - \tilde{b} \). Then the \((k+1)st\) residual is given by the following expression

\[
\tilde{r}_{k+1} = \tilde{r}_k + \alpha_k A\tilde{p}_k.
\]

Proof.

\[
\tilde{r}_{k+1} = A\tilde{x}_{k+1} - \tilde{b} = A(\tilde{x}_k + \alpha_k \tilde{p}_k) - \tilde{b} = \alpha_k A\tilde{p}_k + (A\tilde{x}_k - \tilde{b}) = \alpha_k A\tilde{p}_k + \tilde{r}_k.
\]

We note that the matrix \( (S^T AS) \) is diagonal by the conjugacy property, and that each coordinate direction \( \hat{e}_i \) in \( \hat{x} \)-space corresponds to the direction \( \tilde{p}_{i-1} \) in \( x \)-space.

Before we state a fundamental theorem regarding the conjugate direction method, we show the following lemma:

Lemma

Given a starting point \( \tilde{x}_0 \in \mathbb{R}^n \) and a set of conjugate directions \( \{ \tilde{p}_0, \tilde{p}_1, \ldots, \tilde{p}_{n-1} \} \) if we generate the sequence \( \tilde{x}_k \in \mathbb{R}^n \) by setting

\[
\tilde{x}_{k+1} = \tilde{x}_k + \alpha_k \tilde{p}_k,
\]

where \( \alpha_k = \frac{-\tilde{r}_k^T \tilde{p}_k}{\tilde{p}_k^T \tilde{A} \tilde{p}_k} \),

with \( \tilde{r}_k = A\tilde{x}_k - \tilde{b} \). Then the \((k+1)st\) residual is given by the following expression

\[
\tilde{r}_{k+1} = \tilde{r}_k + \alpha_k A\tilde{p}_k.
\]
Expanding Subspace Minimization: Proof 1 of 3

First, we show that a point \( \tilde{x} \) minimizes \( \Phi \) over the set \( S(\tilde{x}_0, k) \) if and only if \( (\tilde{x})^T \bar{p}_i = 0, \ i = 0, 1, \ldots, k - 1 \).
Let \( h(\tilde{\sigma}) = \Phi(\tilde{x}_0 + \sigma_0 \bar{p}_0 + \sigma_1 \bar{p}_1 + \cdots + \sigma_{k-1} \bar{p}_{k-1}) \). Since \( h(\tilde{\sigma}) \) is a strictly convex quadratic it has a unique minimizer \( \tilde{\sigma}^* \) that satisfies

\[
\frac{\partial h(\tilde{\sigma}^*)}{\partial \sigma_i} = 0, \quad i = 0, 1, \ldots, k - 1
\]

By the chain rule, this is equivalent to

\[
\nabla \Phi(\tilde{x}_0 + \sigma_0 \bar{p}_0 + \sigma_1 \bar{p}_1 + \cdots + \sigma_{k-1} \bar{p}_{k-1})^T \bar{p}_i = 0, \quad i = 0, 1, \ldots, k - 1
\]

We recall that \( \nabla \Phi(\tilde{x}) = \bar{A} \tilde{x} - \bar{b} = \tilde{r}(\tilde{x}) \), thus we have established

\( \tilde{r}(\tilde{x})^T \bar{p}_i = 0 \iff \tilde{x} \) minimizes \( \Phi \) over the set \( S(\tilde{x}_0, k) \).

\( \square \)

Expanding Subspace Minimization: Proof 2 of 3

Proof: Part 2.
We now show that the residuals \( \tilde{r}_k \) satisfy \( \tilde{r}_k^T \bar{p}_i = 0, \ i = 0, 1, \ldots, k - 1 \).
We use mathematical induction. Since \( \alpha_0 \) is always the 1D-minimizer, we have \( \tilde{r}_0^T \bar{p}_0 = 0 \), establishing the base case.

From the inductive hypothesis, that \( \tilde{r}_{k-1}^T \bar{p}_i = 0, \ i = 0, 1, \ldots, k - 2 \), we must show that \( \tilde{r}_k^T \bar{p}_i = 0, \ i = 0, 1, \ldots, k - 1 \) in order to complete the proof.

From the lemma we have an expression for \( \tilde{r}_k = \tilde{r}_{k-1} + \alpha_{k-1} \bar{A} \bar{p}_{k-1} \).
First off we have: \( \bar{p}_{k-1}^T \tilde{r}_k = \bar{p}_{k-1}^T \tilde{r}_{k-1} + \alpha_{k-1} \bar{p}_{k-1}^T \bar{A} \bar{p}_{k-1} = 0 \), since, by construction (optimality)

\[
\alpha_{k-1} = \frac{-\bar{p}_{k-1}^T \tilde{r}_{k-1}}{\bar{p}_{k-1}^T \bar{A} \bar{p}_{k-1}}
\]

Expanding Subspace Minimization: Proof 3 of 3

Proof: Part 3.
Finally,

\[
\tilde{p}_i^T \tilde{r}_k = \tilde{p}_i^T \tilde{r}_{k-1} + \alpha_{k-1} \tilde{p}_i^T \bar{A} \bar{p}_{k-1} = 0, \quad i = 0, 1, \ldots, k - 2
\]

since

\[
\tilde{p}_i^T \tilde{r}_{k-1} = 0, \quad i = 0, 1, \ldots, k - 2
\]

by the induction hypothesis, and

\[
\tilde{p}_i^T \bar{A} \bar{p}_{k-1} = 0, \quad i = 0, 1, \ldots, k - 2
\]

by conjugacy. This establishes \( \tilde{p}_i^T \tilde{r}_k = 0, \ i = 0, 1, \ldots, k - 1 \), which completes the proof.

\( \square \)

Cliff-Hangers...

Cliff-Hanger Questions:

- How can we make this useful?
- Given \( A \), how do we get a set of conjugate vectors? (They are not for sale at Costco!)
- Even if we have them, why is this scheme any better than Gaussian elimination?
- Where is the gradient?
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