Conjugate gradient method

$A \in \mathbb{R}^{n \times n}$ positive definite

$b \in \mathbb{R}^n$

$$Ap = b \iff \min_{p \in \mathbb{R}^n} \frac{1}{2} p^T A p - b^T p$$

Inner product on $\mathbb{R}^n$

$x, y \in \mathbb{R}^n$ $\quad \langle x, y \rangle = x^T y = \sum_{i=1}^{n} x_i y_i$

An inner product on $\mathbb{R}^n$ is a function

$$F : \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathbb{R}$$

$$(x, y) \longrightarrow F(x, y) \quad \text{s.t.}$$

1) $F(x_1 + x_2, y) = F(x_1, y) + F(x_2, y)$
2) $F(x, y) = F(y, x)$
3) $F(\alpha x, y) = \alpha F(x, y) \quad \forall \alpha \in \mathbb{R}$
4) $F(x, x) \geq 0$ and $F(x, x) = 0$ iff $x = 0$

Ex 1: Standard "dot product"

$F(x, y) = \sum_{i=1}^{N} x_i y_i$ is an inner product

Ex 2: $A \in \mathbb{R}^{n \times n}$ positive definite

$$F(x, y) = x^T A y \Rightarrow \langle x, y \rangle_A$$

let $F: \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathbb{R}$ be any inner product

$\exists A$ PSD s.t. $F(x,y) = \langle x, y \rangle_A$

$\hookrightarrow$ basis vector $\quad A_{ij} = \langle e_i, e_j \rangle$

Def: ① let $\langle \cdot, \cdot \rangle_A$ be some inner product

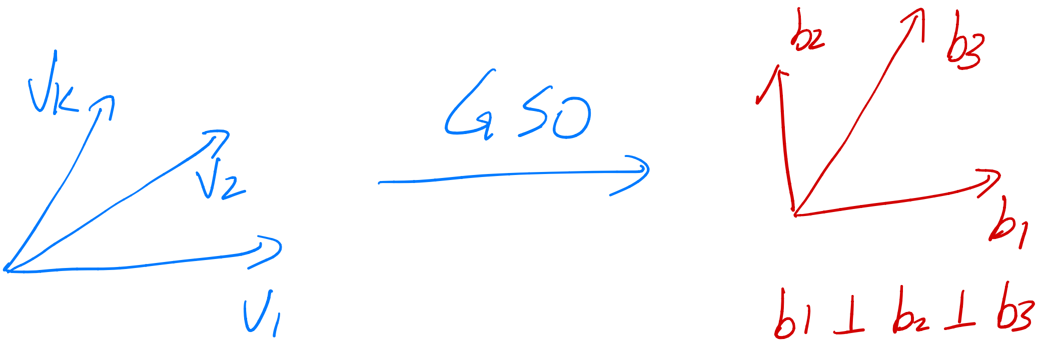
$x \perp y$ if $\langle x, y \rangle_A = 0$

② $L \subseteq \mathbb{R}^n$ linear subspace of $\mathbb{R}^n$

$L_A^{\perp} := \{ y \in \mathbb{R}^n : \langle x, y \rangle_A = 0, \ \forall x \in L \}$

$\rightarrow$ x and y are said to be A-conjugate

Gram-Schmidt Orthogolisation (GSO)



$b_1 \perp b_2 \perp b_3$

$\text{span}(V_1, V_2, V_3) = \text{span}(b_1, b_2, b_3)$ same subspace

Def: $x, y \in \mathbb{R}^n$, The projection of x into y with respect to the inner product $\langle \cdot , \cdot \rangle_A$ is

$$\left(\frac{\langle x, y \rangle_A}{\langle y, y \rangle_A} \right) \cdot y$$

GSO procedure:

Input: $v_1, \cdots v_k$ linearly independent

Output: $b_1, \cdots b_k$ s.t.

implie

① $\langle b_i, b_j \rangle_A = 0$ if $i=j$ (mutually orthorgonal)

② $\text{span}(b_1, \cdots, b_i) = \text{span}(v_1, \cdots, v_i)$
$\forall i = 1, 2, \cdots, k$

1. set $b_1 = v_1$

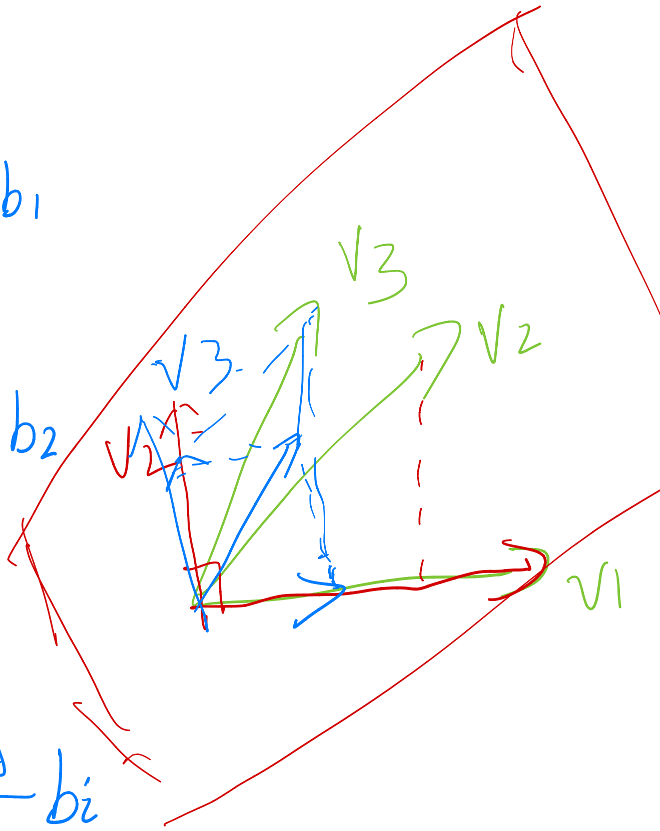
2. $i = 1, \cdots, k-1$

$$b_{i+1} = V_{i+1} - \frac{\langle V_{i+1}, b_1 \rangle_A}{\langle b_1, b_1 \rangle_A} b_1$$

$$- \frac{\langle V_{i+1}, b_2 \rangle_A}{\langle b_2, b_2 \rangle_A} b_2$$

$$\vdots$$

$$- \frac{\langle V_{i+1}, b_i \rangle_A}{\langle b_i, b_i \rangle_A} b_i$$



Projection of V_3 into $\text{span}(b_1, b_2)$ = Projection of V_3 into b_1 + Projection of V_3 into b_2
$(b_1 \perp b_2)$

$$\min_{p \in \mathbb{R}^n} \frac{1}{2} p^T A p - b^T p$$

$$= \frac{1}{2} \langle p, p \rangle_A - b^T p$$

$$\boxed{\text{Suppose we have a } A\text{-conjugate basis } s_1, \cdots, s_n \text{ for } \mathbb{R}^n}$$

$$p = \lambda_1 s_1 + \cdots + \lambda_n s_n \quad (s_1, \cdots s_n \text{ span } \mathbb{R}^n)$$

$$\frac{1}{2} \langle \lambda_1 s_1 + \cdots + \lambda_n s_n, \lambda_1 s_1 + \cdots + \lambda_n s_n \rangle_A - b^T (\lambda_1 s_1 + \cdots + \lambda_n s_n)$$

$$= \frac{1}{2} \lambda_1^2 \langle s_1, s_1 \rangle_A + \frac{1}{2} \lambda_2^2 \langle s_2, s_2 \rangle + \cdots + \frac{1}{2} \lambda_n^2 \langle s_n, s_n \rangle$$

$$- \lambda_1 b^T s_1 - \lambda_2 b^T s_2 - \cdots - \lambda_n b^T s_n$$

$$\min_{\lambda_1 \cdots \lambda_n} \frac{1}{2} \underbrace{\langle s_1, s_1 \rangle_A}_{a_1} \lambda_1^2 - \underbrace{(b^T s_1)}_{b_1} \lambda_1$$

$$+ \frac{1}{2} \underbrace{\langle s_2, s_2 \rangle_A}_{a_2} \lambda_2^2 - \underbrace{(b^T s_2)}_{b_2} \lambda_2$$

$$\vdots$$

$$+ \frac{1}{2} \underbrace{\langle s_n, s_n \rangle_A}_{a_n} \lambda_n^2 - \underbrace{(b^T s_n)}_{b_n} \lambda_n$$

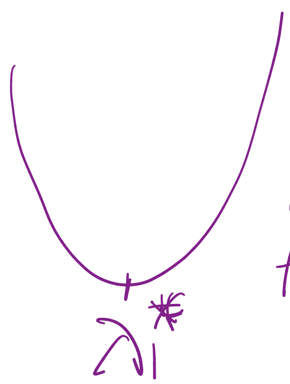
$$b_i = b^T s_i$$

$$a_i = \langle s_i, s_i \rangle_A$$

$$\min_{\lambda_1 \cdots \lambda_n \in \mathbb{R}} \left(\frac{1}{2} a_1 \lambda_1^2 - b_1 \lambda_1\right) + \left(\frac{1}{2} a_2 \lambda_2^2 - b_2 \lambda_2\right) + \cdots \left(\frac{1}{2} a_n \lambda_n - b_n \lambda_n\right)$$

$$\min_{\lambda_1 \in \mathbb{R}} \frac{1}{2} a_1 \lambda_1^2 - b_1 \lambda_1 \quad (a_1 > 0)$$

$$\lambda_1^* = \frac{b_1}{a_1}$$



convex function

Optimal Solution: $\left(\frac{b_1}{a_1}, \frac{b_2}{a_2}, \cdots \frac{b_n}{a_n}\right)$

$\lambda_1, \lambda_2, \cdots \lambda_n$

$$p = \lambda_1 s_1 + \cdots + \lambda_n s_n$$

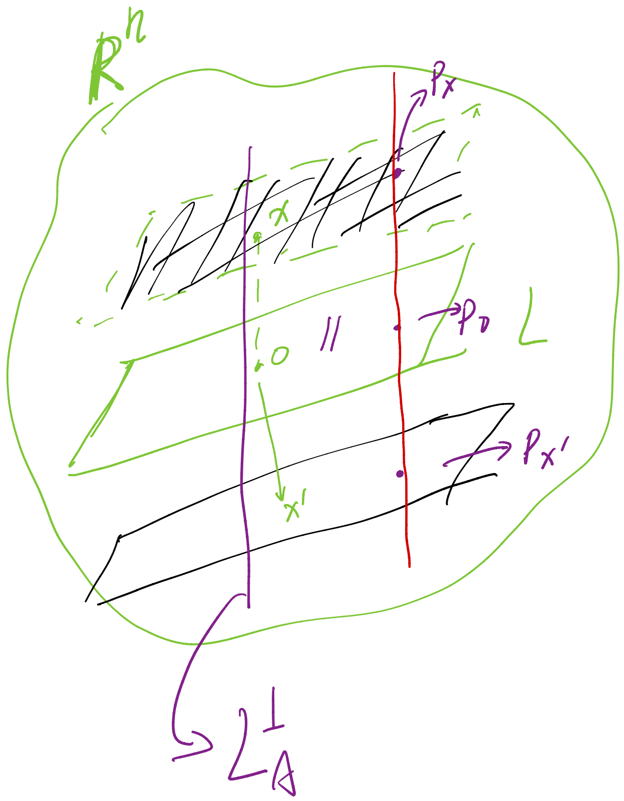
$$\boxed{p = \frac{b_1}{a_1} s_1 + \cdots + \frac{b_n}{a_n} s_n}$$

A is symetric positive definite

$$F_{A,b}(p) = \frac{1}{2} p^T A p - b^T p$$

Theorem: $L \in \mathbb{R}^n$ linear subspace of $\mathbb{R}^n$

parallel translate of L: $x + L$ for some $x \in \mathbb{R}^n$



Consider the minimizer $F_{A,b}(p)$ restricted to this translate

- These minimizer together form a translate of $L_A^\perp$

$L = \text{span}(s_1, s_2, \cdots, s_k)$

$L \in \mathbb{R}^n$ but $L \neq \mathbb{R}^n$

proof: let $s_1, s_2, \cdots, s_k$ be A-conjugate basis of L

Find $s_{k+1}, \cdots s_n$ s.t. $s_1, s_2, \cdots s_n$ form an A-conjugate basis of $\mathbb{R}^n$

① Find the conjugate complement (orthorgornal) of L and do GSO

② Find a vector outside L and do GSO to check if it's within L until they span $\mathbb{R}^n$

Claim: $s_{k+1}, \cdots s_n$ are basis for $L_A^\perp$

$$F_{A,b}(p) = \frac{1}{2}\langle s_1, s_1\rangle_A \lambda_1^2 + \cdots + \frac{1}{2}\langle s_n, s_n\rangle_A \lambda_n^2$$
$$- b^T s_1 \lambda_1 - \cdots - b^T s_n \lambda_n$$

Translate of L: setting some arbitrary value to $\overline{\lambda_{k+1}}, \cdots \overline{\lambda_n}$

$(L = \mathrm{span}(s_1, \cdots, s_k))$

and now we minimize $\lambda_1, \cdots, \lambda_k$

$$\lambda_1 = \frac{\langle s_1, s_1\rangle_A}{b^T s_1} \quad \cdots \quad \lambda_k = \frac{\langle s_k, s_k\rangle_A}{b^T s_k}$$

Translate of L decided by $\lambda_{k+1}, \cdots \lambda_n$ / with fixed $\lambda_1, \cdots \lambda_k$

$\mathrm{span}(s_1, \cdots s_k) = L$

Translate of $L_A^\perp$ decided by $\lambda_1, \cdots \lambda_k$ / with fixed $\lambda_{k+1}, \cdots \lambda_n$

$\mathrm{span}(s_{k+1}, \cdots, s_n) = L_A^\perp$

$L \cap L_A^{\perp}$ = origin zero vector

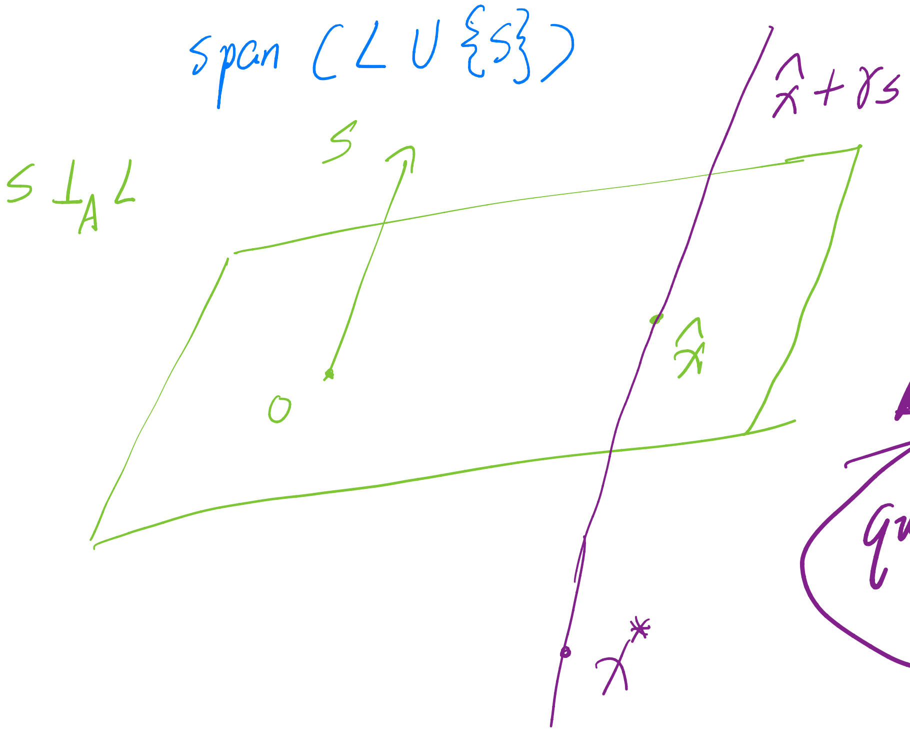
Eigenvectors of A are not supposed to be basis of A-conjugate basis. Because they might not be orthorgonal to each other

Theorem: $L \subseteq \mathbb{R}^n$ linear subspace $s \in \mathbb{R}^n$ s.t.

$s \perp_A L \quad (s \in L_A^{\perp})$

let $\hat{x}$ be the minimizer of $F_{A,b}$, restricted to L, let x^* be the minimizer of $F_{A,b}$, restricted to line $\{\hat{x} + \gamma s, \gamma \in \mathbb{R}\}$

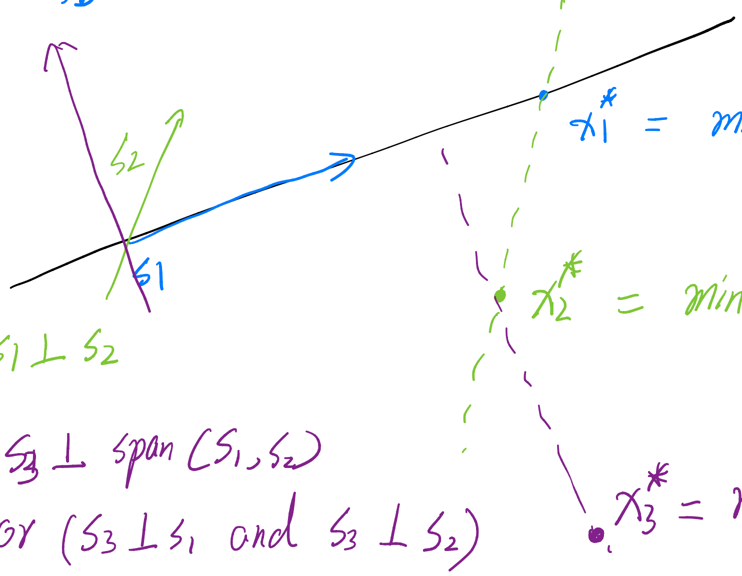
Then, x^* is the minimizer of $F_{A,b}$, restricted to span $(L \cup \{s\})$



Quadratic Convex function

Reason behind

$F_{A,b}$



$s_1 \perp s_2$

$x_1^* = \text{minimizer of } F_{A,b} \text{ in } \vec{s}_1$

$x_2^* = \text{minimizer of } F_{A,b} \text{ in } x_1^* + \gamma \vec{s}_2$

$\text{span}(\vec{s}_1, \vec{s}_2)$

$s_3 \perp \text{span}(s_1, s_2)$

or $(s_3 \perp s_1 \text{ and } s_3 \perp s_2)$

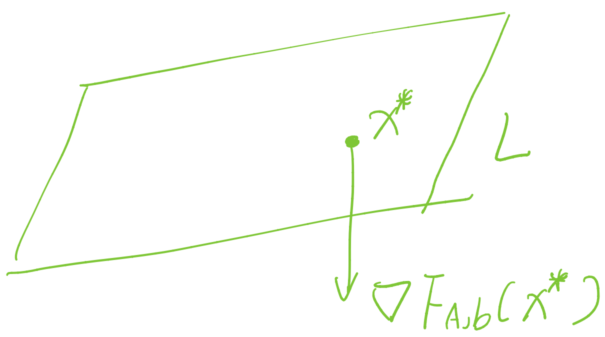
$x_3^* = \text{minimizer of } F_{A,b} \text{ in } x_2^* + \gamma \vec{s}_3$

$\text{span}(\vec{s}_1, \vec{s}_2, \vec{s}_3)$

The reason why we can do this Because $F_{A,b}$ is a quadratic convex function (can consider it as find minimum at each $x^* + \gamma \vec{s}_k$ – axis) and $s_1, \dots s_n$ are mutually orthorgonal (linearly independent)

Lemma: $L \subseteq \mathbb{R}^n$ linear subspace, let x^* be the minimizer of $F_{A,b}$, restricted to L.

$\nabla F_{A,b}(x^*) \neq 0$ $\quad \nabla F_{A,b}(x^*) \perp_{\text{Standard Inner Product}} L$



Fact: $F_{A,b}(p) = \frac{1}{2} p^T A p - b^T p$

$\nabla F_{A,b}(\bar{p}) = A\bar{p} - b$

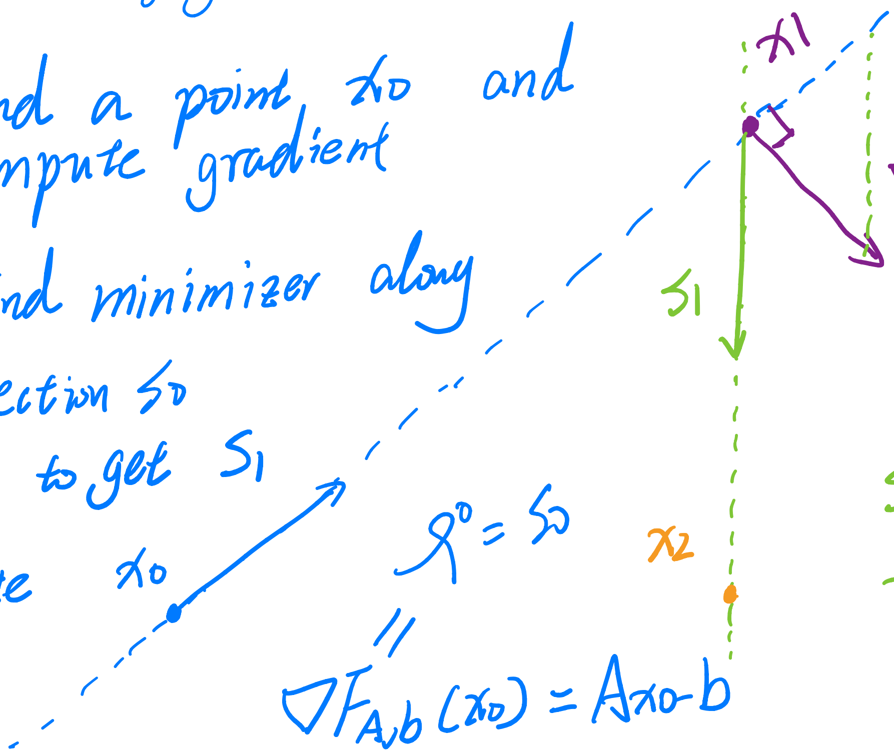
Improve conjugate Gradient

① Find a point x_0 and compute gradient

② Find minimizer along direction s_0

③ GSO to get s_1

④ repeate



s_1 is A-conjugate to s_0

$\langle s_1, s_0 \rangle_A = 0$

Algorithm:

① Initialize x_0, $s_0 = \nabla F_{A,b}(x_0) = r_0$

② for $i = 0, \cdots, n-1$:

a) compute α_i s.t. $x_i + \alpha_i s_i$ is the minimizer on $\{x_i + \alpha s_i;\ \alpha_i \in \mathbb{R}\}$

b) $x_{i+1} = x_i + \alpha_i s_i$

c) $g^{i+1} = \nabla F_{A,b}(x_{i+1}) = Ax_{i+1} - b$

d) $s_{i+1} = g^{i+1} - \sum_{j=1}^{i} \frac{\langle r_{i+1}, s_j \rangle_A}{\langle s_j, s_j \rangle_A} s_j$

$= g^{i+1} - \frac{\langle g^{i+1}, s_i \rangle_A}{\langle s_i, s_i \rangle_A} s_i$ IT SAVE A LOT !!!

($\nabla F_{A,b}(x_{i+1}) = g^{i+1}$ must orthogonal to previous $0 \sim i-1$)

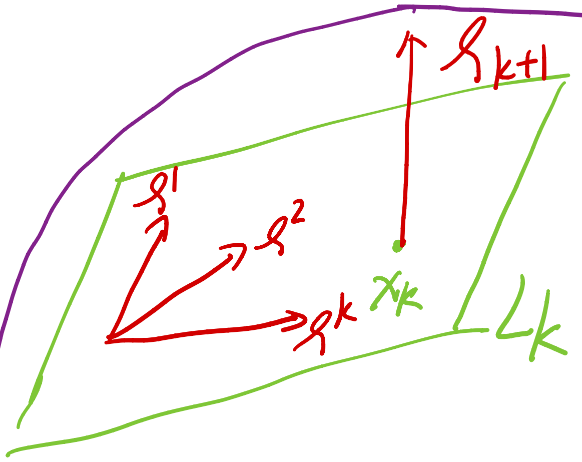
Lemma: $\forall k = 0, 1, \cdots n$

$\text{span}\{g_0, g_1, g_2 \cdots\} = \text{span}\{s_0, s_1, \cdots\}$

Theorem: $\forall k = 0, 1, \cdots, n-1,$

Then $\langle g^k, s^j \rangle_A = 0$ if $0 \le j \le k-1$

$\langle g^{k+1}, g^j \rangle = 0 \quad \forall 0 \le j \le k-1$



$(g^{k+1})^T A s^j \rightarrow$ Recall: $x^{j+1} = x^j + \alpha_j s^j$

$\Rightarrow s^j = \frac{1}{\alpha_j}(x^{j+1} - x^j)$

$\Rightarrow (g^{k+1})^T A \cdot [\frac{1}{\alpha_j}(x^{j+1} - x^j)]$

$$= \frac{1}{\alpha_j} (g^{k+1})^T (A x^{j+1} - A x^j)$$

$$= \frac{1}{\alpha_j} (g^{k+1})^T \left[(A x^{j+1} - b) - (A x^j - b) \right]$$

$g^{i+1} \perp L_k$

$$= \frac{1}{\alpha_j} (g^{k+1})^T (g^{j+1} - g^j)$$

$$= 0 \quad \text{if } j \le k-1$$

Step 2a:

$\hat{x}$, $\hat{s}$

$$\underset{\alpha \in \mathbb{R}}{\text{minimizing}} \; F_{A,b}(\hat{x} + \alpha \hat{s})$$

$$\min_{\alpha} \frac{1}{2} (\hat{x} + \alpha \hat{s})^T A (\hat{x} + \alpha \hat{s}) - b^T (\hat{x} + \alpha \hat{s})$$

$$\Rightarrow \min_{\alpha} \frac{1}{2} \alpha^2 \langle \hat{s}, \hat{s} \rangle_A + \frac{1}{2} \alpha \langle \hat{s}, \hat{x} \rangle_A + \frac{1}{2} \langle \hat{x}, \hat{x} \rangle_A - b^T \hat{x} - \alpha b^T \hat{s}$$

$$\Rightarrow \min_{\alpha} c_1 \alpha^2 - c_2 \alpha + c_3$$

$$\lambda^* = \frac{\hat{s}^T (b - A\hat{x})}{\langle \hat{s}, \hat{s} \rangle_A}$$

$$\overset{n\times n}{M} \cdot \overset{n\times 1}{x}$$

$$O(n \cdot T(\underbrace{n \times n \text{ matrix with } n \text{ vector}}_{n^2}))$$

$= O(n^3)$ ← Gaussian elimination

if A is sparse. $n^2 \to k \cdot n$

$= O(kn^2)$

The conjugate gradient method

Amitabh Basu

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1 Inner products on Euclidean space

The notion of an abstract inner product on $\mathbb{R}^n$ is useful in making the idea behind the "Conjugate Gradient Method" transparent. Thus, we begin with defining what a general inner product is.

Definition 1.1. An *inner product on* $\mathbb{R}^n$ is any function $\langle\cdot,\cdot\rangle : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ that satisfies the following conditions.

1. (Nonnegativity) $\langle \mathbf{x}, \mathbf{x}\rangle \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$. Moreover, $\langle \mathbf{x}, \mathbf{x}\rangle = 0$ if and only if $\mathbf{x} = 0$.
2. (Symmetry) $\langle \mathbf{x}, \mathbf{y}\rangle = \langle \mathbf{y}, \mathbf{x}\rangle$.
3. (Bilinearity – vector addition) $\langle \mathbf{x} + \mathbf{y}, \mathbf{z}\rangle = \langle \mathbf{x}, \mathbf{z}\rangle + \langle \mathbf{y}, \mathbf{z}\rangle$.
4. (Bilinearity – scalar multiplication) $\langle \alpha\mathbf{x}, \mathbf{y}\rangle = \alpha\langle \mathbf{x}, \mathbf{y}\rangle$.

Example 1.2. Let $A \in \mathbb{R}^{n\times n}$ be a positive definite matrix. Then $\langle \mathbf{x}, \mathbf{y}\rangle_A := \mathbf{x}^T A\mathbf{y}$ is an inner product.

Theorem 1.3. Any inner product on $\mathbb{R}^n$ is of the form $\langle \mathbf{x}, \mathbf{y}\rangle_A$ for some positive definite matrix A.

Proof. Consider an arbitrary inner product $\langle\cdot,\cdot\rangle$ on $\mathbb{R}^n$. Define the matrix $A_{ij} := \langle e^i, e^j\rangle$, where e^i, $i = 1, \ldots, n$ denotes the standard unit vector. It is not hard to verify, using the properties of the inner product, that $\langle \mathbf{x}, \mathbf{y}\rangle = \mathbf{x}^T A\mathbf{y}$. $\square$

In the following, we will always index an inner product with a positive definite matrix A, unless we mean the standard inner product on $\mathbb{R}^n$, i.e., A is the identity matrix. In this case, we will not have any subscript.

Definition 1.4. (Orthogonality) Any inner product on $\mathbb{R}^n$ gives a notion of "orthogonal vectors". We define the following:

1. We say that $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ are *orthogonal with respect to the inner product* $\langle \cdot, \cdot \rangle_A$ if $\langle \mathbf{x}, \mathbf{y} \rangle_A = 0$. We also say that $\mathbf{x}$ and $\mathbf{y}$ are *A-conjugate*.

2. Let $L \subseteq \mathbb{R}^n$ be a linear subspace. Then the *orthogonal complement of L with respect to* $\langle \cdot, \cdot \rangle_A$ is defined as $L_A^\perp := \{\mathbf{y} \in \mathbb{R}^n : \langle \mathbf{x}, \mathbf{y} \rangle_A = 0 \quad \forall \mathbf{x} \in L\}$. We also say that $L_A^\perp$ is the *A-conjugate subspace* of L.

1.1 Gram-Schmidt orthogonolization

Definition 1.5. Given $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and an inner product $\langle \cdot, \cdot \rangle_A$, we say that the projection of $\mathbf{x}$ on $\mathbf{y}$ with respect to $\langle \cdot, \cdot \rangle_A$ is given by $\frac{\langle \mathbf{x}, \mathbf{y} \rangle_A}{\langle \mathbf{y}, \mathbf{y} \rangle_A} \mathbf{y}$.

Lemma 1.6. Let $\mathbf{x}^1, \ldots, \mathbf{x}^k$ be pairwise A-conjugate for some positive definite matrix A. Then $\mathbf{x}^1, \ldots, \mathbf{x}^k$ are all linearly independent. Moreover, for any $\mathbf{x} \in \mathrm{span}(\mathbf{x}^1, \ldots, \mathbf{x}^k)$, the unique decomposition of $\mathbf{x}$ as a linear combination of $\mathbf{x}^1, \ldots, \mathbf{x}^k$ is given by $\mathbf{x} = \frac{\langle \mathbf{x}, \mathbf{x}^1 \rangle_A}{\langle \mathbf{x}^1, \mathbf{x}^1 \rangle_A} \mathbf{x}^1 + \frac{\langle \mathbf{x}, \mathbf{x}^2 \rangle_A}{\langle \mathbf{x}^2, \mathbf{x}^2 \rangle_A} \mathbf{x}^2 + \ldots + \frac{\langle \mathbf{x}, \mathbf{x}^k \rangle_A}{\langle \mathbf{x}^k, \mathbf{x}^k \rangle_A} \mathbf{x}^k$. In other words, $\mathbf{x}$ is the sum of the projections of $\mathbf{x}$ onto $\mathbf{x}^1, \ldots, \mathbf{x}^k$.

Gram-Schmidt Orthogonalization procedure. INPUT: A positive definite matrix A and a set of linearly independent vectors $\mathbf{x}^1, \ldots, \mathbf{x}^k$ $(1 \leq k \leq n)$.

OUTPUT: A set $\mathbf{b}^1, \ldots, \mathbf{b}^k$ that are pairwise A-conjugate with respect to a given positive definite matrix A such that the following holds for all $i = 1, \ldots, k$: $\mathrm{span}(\mathbf{b}^1, \ldots, \mathbf{b}^i) = \mathrm{span}(\mathbf{x}^1, \ldots, \mathbf{x}^i)$.

1. Let $\mathbf{b}^1 = \mathbf{x}^1$.

2. For $i = 1, \ldots, k-1$, set
$$\mathbf{b}_{i+1} := \mathbf{x}^{i+1} - \sum_{j=1}^{i} \frac{\langle \mathbf{x}^{i+1}, \mathbf{b}^j \rangle_A}{\langle \mathbf{b}^j, \mathbf{b}^j \rangle_A} \mathbf{b}^j.$$

2 Conjugate Gradient Method

2.1 Minimizing a convex quadratic using A-conjugate vectors

Let $A \in \mathbb{R}^{n \times n}$ be a positive definite matrix and $\mathbf{b} \in \mathbb{R}^n$. We would like to solve the convex, quadratic minimization problem
$$\min_{\mathbf{p} \in \mathbb{R}^n} \frac{1}{2} \mathbf{p}^T A \mathbf{p} - \mathbf{b}^T \mathbf{p} = \min_{\mathbf{p} \in \mathbb{R}^n} \frac{1}{2} \langle \mathbf{p}, \mathbf{p} \rangle_A - \mathbf{b}^T \mathbf{p}.$$

Equivalently, we want to solve the system
$$A\mathbf{p} = \mathbf{b}.$$

The main observation is that if $\{\mathbf{s}^1, \ldots, \mathbf{s}^n\}$ are any pairwise A-conjugate vectors, then the problem becomes easier to solve in this basis. In particular, write $\mathbf{p} = \lambda_1 \mathbf{s}^1 + \ldots + \lambda_n \mathbf{s}^n$. The objective then becomes

$$\frac{1}{2}\langle \mathbf{p}, \mathbf{p}\rangle_A - \mathbf{b}^T\mathbf{p} = \lambda_1^2 \frac{\langle \mathbf{s}^1, \mathbf{s}^1\rangle_A}{2} + \lambda_2^2 \frac{\langle \mathbf{s}^2, \mathbf{s}^2\rangle_A}{2} + \ldots + \lambda_n^2 \frac{\langle \mathbf{s}^n, \mathbf{s}^n\rangle_A}{2} - \lambda_1(\mathbf{b}^T\mathbf{s}^1) - \lambda_2(\mathbf{b}^T\mathbf{s}^2) - \ldots - \lambda_n(\mathbf{b}^T\mathbf{s}^n).$$

Thus, we are now minimizing

$$\min_{\lambda_1, \ldots, \lambda_n} \frac{a_1}{2}\lambda_1^2 + \ldots + \frac{a_n}{2}\lambda_n^2 - b_1\lambda_1 - \ldots - b_n\lambda_n,$$

where $a_1, \ldots, a_n > 0$ and $b_1, \ldots, b_n \in \mathbb{R}$. This is an easy problem to solve because the λ's do not interact with each other. In other words, we can set $\bar{\lambda}_i = \frac{b_i}{a_i}$ and the solution is $\overline{\mathbf{p}} = \bar{\lambda}_1 \mathbf{s}^1 + \ldots + \bar{\lambda}_n \mathbf{s}^n$.

A nice consequence of the above observations is the following.

Theorem 2.1. Let $A \in \mathbb{R}^{n\times n}$ be a positive definite matrix and $\mathbf{b} \in \mathbb{R}^n$. Define $f(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T A\mathbf{p} - \mathbf{b}^T\mathbf{p}$. Let L be an arbitrary linear subspace of $\mathbb{R}^n$. Consider all possible translates of this linear subspace, i.e., $L_{\mathbf{x}} := \mathbf{x} + L$ for $\mathbf{x} \in \mathbb{R}^n$. For any such translate $L_{\mathbf{x}}$, consider the minimizer of f restricted to $L_{\mathbf{x}}$. Then the set of all such minimizers forms a translate of $L_A^\perp$.

Proof. By the Gram-Schmidt process, one can find a basis $\{\mathbf{s}^1, \ldots, \mathbf{s}^k\}$ of L such that these vectors are pairwise A-conjugate. Moreover, this basis can be completed to a basis of $\mathbb{R}^n$; let this basis be $\{\mathbf{s}^1, \ldots, \mathbf{s}^k, \mathbf{s}^{k+1}, \ldots, \mathbf{s}^n\}$. Note that $L_A^\perp$ is precisely the span of $\{\mathbf{s}^k, \mathbf{s}^{k+1}, \ldots, \mathbf{s}^n\}$. □

2.2 Finding A-conjugate vectors.

We have thus reduced the problem to finding A-conjugate vectors. By the Gram-Schmidt process described above, we can start with an arbitrary basis of $\mathbb{R}^n$ – for example, the standard unit vectors $\mathbf{e}^1, \ldots, \mathbf{e}^n$ – and produce a set of A-conjugate vectors using the Gram-Schmidt process. But this involves taking many matrix-vector products. We will now show that if we pick a suitably chosen set of linear independent vectors, then a significant savings in computation can be achieved.

Lemma 2.2. Let $\mathbf{x}^0$ be an arbitrary point in $\mathbb{R}^n$ and let L be any linear subspace of $\mathbb{R}^n$. Let $\bar{\mathbf{x}}$ be the minimizer of the function $f(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T A\mathbf{p} - \mathbf{b}^T\mathbf{p}$ restricted to $\mathbf{x}^0 + L$. Then $\nabla f(\bar{\mathbf{x}}) = A\bar{\mathbf{x}} - \mathbf{b}$ is orthogonal to L with respect to the standard inner product on $\mathbb{R}^n$.

Lemma 2.3. Let $\mathbf{x}^0$ be an arbitrary point in $\mathbb{R}^n$ and let L be any linear subspace of $\mathbb{R}^n$. Let $\bar{\mathbf{x}}$ be the minimizer of the function $f(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T A\mathbf{p} - \mathbf{b}^T\mathbf{p}$ restricted to $\mathbf{x}^0 + L$. Let $\mathbf{s} \in \mathbb{R}^n$ be any vector that is A-conjugate to L. Let $\hat{\mathbf{x}}$ be the minimizer of the one-dimensional function obtained by restricting f to the line $\{\bar{\mathbf{x}} + \alpha\mathbf{s} : \alpha \in \mathbb{R}\}$. Then $\hat{\mathbf{x}}$ is the minimizer of f restricted to $\mathbf{x}^0 + \mathrm{span}(L \cup \{\mathbf{s}\})$.

We now describe a specialized, iterative way of choosing the A-conjugate vectors:

Conjugate Gradient method: Basic.

1. Initialize an arbitrary $\mathbf{x}^0 \in \mathbb{R}^n$. Let $\mathbf{s}^0 = \mathbf{r}^0 = \mathbf{b} - A\mathbf{x}^0 = -\nabla f(\mathbf{x}^0)$.

2. For $i = 0, 1, \ldots, n-1$

   (a) Minimize the one-dimensional function $\phi(\alpha) = f(\mathbf{x}^i + \alpha \mathbf{s}^i)$; let α_i be the minimizer.

   (b) Set $\mathbf{x}^{i+1} := \mathbf{x}^i + \alpha_i \mathbf{s}^i$.

   (c) Set $\mathbf{r}^{i+1} := -\nabla f(\mathbf{x}^{i+1}) = \mathbf{b} - A\mathbf{x}^{i+1}$.

   (d) Set $\mathbf{s}^{i+1} := \mathbf{r}^{i+1} - \sum_{j=0}^{i} \frac{\langle \mathbf{r}^{i+1}, \mathbf{s}^j \rangle_A}{\langle \mathbf{s}^j, \mathbf{s}^j \rangle_A} \mathbf{s}^j$.

Lemma 2.4. Let $\{\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^{k+1}\}$, $\{\mathbf{r}^0, \ldots, \mathbf{r}^{k+1}\}$, and $\{\mathbf{s}^0, \ldots, \mathbf{s}^{k+1}\}$ be the sequence of vectors generated in the algorithm above for some $0 \leq k \leq n-1$. Then the following hold:

(i) $\mathrm{span}(\{\mathbf{r}^0, \ldots, \mathbf{r}^k\}) = \mathrm{span}(\{\mathbf{s}^0, \ldots, \mathbf{s}^k\})$.

(ii) $\mathbf{x}^{k+1}$ is minimizer of f restricted to $\mathbf{x}^0 + \mathrm{span}(\{\mathbf{r}^0, \ldots, \mathbf{r}^k\})$.

Proof. Part (i) follows from the Gram-Schmidt procedure. We prove part (ii) by induction on k. For $k = 1$, the result follows from definition of $\mathbf{x}^1$. Lemma 2.3 and the induction hypothesis completes the induction step. □

Lemma 2.5. Let $\{\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^{k+1}\}$, $\{\mathbf{r}^0, \ldots, \mathbf{r}^{k+1}\}$, and $\{\mathbf{s}^0, \ldots, \mathbf{s}^{k+1}\}$ be the sequence of vectors generated in the algorithm above for some $1 \leq k \leq n-1$. Then $\langle \mathbf{r}^{k+1}, \mathbf{s}^j \rangle_A = 0$ for all $0 \leq j \leq k-1$.

Proof. By Lemma 2.4 (i), $\mathrm{span}(\{\mathbf{r}^0, \ldots, \mathbf{r}^j\}) = \mathrm{span}(\{\mathbf{s}^0, \ldots, \mathbf{s}^j\})$ for all $0 \leq j \leq k+1$. Let this linear space be denoted by L_j. By Lemma 2.4 (i), $\mathbf{x}^{k+1}$ is the minimizer for f restricted to $\mathbf{x}^0 + L_k$. By Lemma 2.2, $\mathbf{r}^{k+1}$ is orthogonal to L_k with respect to the standard inner product. In other words, $(\mathbf{r}^{k+1})^T \mathbf{r}^j = 0$ for all $0 \leq j \leq k$. Now consider

$$\begin{array}{rcl} \langle \mathbf{r}^{k+1}, \mathbf{s}^j \rangle_A & = & (\mathbf{r}^{k+1})^T A \mathbf{s}^j \\ & = & \frac{1}{\alpha_j} (\mathbf{r}^{k+1})^T A (\mathbf{x}^{j+1} - \mathbf{x}^j) \\ & = & \frac{1}{\alpha_j} (\mathbf{r}^{k+1})^T ((\mathbf{b} - A\mathbf{x}^j) - (\mathbf{b} - A\mathbf{x}^{j+1})) \\ & = & \frac{1}{\alpha_j} (\mathbf{r}^{k+1})^T (\mathbf{r}^j - \mathbf{r}^{j+1}) \end{array} \tag{2.1}$$

The last term is 0 for all $j \leq k-1$. □

One can also give a closed form formula for α_i at every iteration of the above algorithm.

Lemma 2.6. Given any $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{s} \in \mathbb{R}^n$, the minimizing $\alpha \in \mathbb{R}$ for $\phi(\alpha) = f(\mathbf{x} + \alpha \mathbf{s})$ is given by $\alpha = \frac{\mathbf{s}^T(\mathbf{b} - A\mathbf{x})}{\langle \mathbf{s}, \mathbf{s} \rangle_A}$.

Conjugate Gradient method: Improved.

1. Initialize an arbitrary $\mathbf{x}^0 \in \mathbb{R}^n$. Let $\mathbf{s}^0 = \mathbf{r}^0 = \mathbf{b} - A\mathbf{x}^0 = -\nabla f(\mathbf{x}^0)$.
2. For $i = 0, 1, \ldots, n-1$
   (a) Set $\alpha_i = \frac{(\mathbf{s}^i)^T \mathbf{r}^i}{\langle \mathbf{s}^i, \mathbf{s}^i \rangle_A}$.
   (b) Set $\mathbf{x}^{i+1} := \mathbf{x}^i + \alpha_i \mathbf{s}^i$.
   (c) Set $\mathbf{r}^{i+1} := -\nabla f(\mathbf{x}^{i+1}) = \mathbf{b} - A\mathbf{x}^{i+1}$.
   (d) Set $\mathbf{s}^{i+1} := \mathbf{r}^{i+1} - \frac{\langle \mathbf{r}^{i+1}, \mathbf{s}^i \rangle_A}{\langle \mathbf{s}^i, \mathbf{s}^i \rangle_A} \mathbf{s}^i$.

One can reduce the number of matrix-vector products from two to one per iteration as follows:

Conjugate Gradient method: Final.

1. Initialize an arbitrary $\mathbf{x}^0 \in \mathbb{R}^n$. Let $\mathbf{s}^0 = \mathbf{r}^0 = \mathbf{b} - A\mathbf{x}^0 = -\nabla f(\mathbf{x}^0)$.
2. For $i = 0, 1, \ldots, n-1$
   (a) Set $\alpha_i = \frac{(\mathbf{r}^i)^T \mathbf{r}^i}{\langle \mathbf{s}^i, \mathbf{s}^i \rangle_A}$.
   (b) Set $\mathbf{x}^{i+1} := \mathbf{x}^i + \alpha_i \mathbf{s}^i$.
   (c) Set $\mathbf{r}^{i+1} := \mathbf{r}^i - \alpha_i A\mathbf{s}^i$.
   (d) Set $\mathbf{s}^{i+1} := \mathbf{r}^{i+1} + \frac{(\mathbf{r}^{i+1})^T \mathbf{r}^{i+1}}{(\mathbf{r}^i)^T \mathbf{r}^i} \mathbf{s}^i$.

Proof of correctness of Final version. First note that in Step 2(c),

$$\mathbf{r}^{i+1} = \mathbf{b} - A\mathbf{x}^{i+1} = \mathbf{b} - A(\mathbf{x}^i + \alpha_i \mathbf{s}^i) = \mathbf{r}^i - \alpha_i A\mathbf{s}^i \tag{2.2}$$

where we used Step 2(b). Next observe that $\alpha_0 = \frac{(\mathbf{s}^0)^T \mathbf{r}^0}{\langle \mathbf{s}^0, \mathbf{s}^0 \rangle_A} = \frac{(\mathbf{r}^0)^T \mathbf{r}^0}{\langle \mathbf{s}^0, \mathbf{s}^0 \rangle_A}$ since $\mathbf{s}^0 = \mathbf{r}^0$. We will show that in every iteration, the equality

$$\alpha_i = \frac{(\mathbf{s}^i)^T \mathbf{r}^i}{\langle \mathbf{s}^i, \mathbf{s}^i \rangle_A} = \frac{(\mathbf{r}^i)^T \mathbf{r}^i}{\langle \mathbf{s}^i, \mathbf{s}^i \rangle_A} \tag{2.3}$$

is maintained. From (2.1), setting $j = k$, we obtain that

$$\langle \mathbf{r}^{k+1}, \mathbf{s}^k \rangle_A = \frac{1}{\alpha_j} (\mathbf{r}^{k+1})^T (\mathbf{r}^k - \mathbf{r}^{k+1}) = -\frac{1}{\alpha_k} (\mathbf{r}^{k+1})^T \mathbf{r}^{k+1}$$

Thus, iteratively, combining this with (2.3), we obtain that in Step 2(d) we have

$$\mathbf{s}^{i+1} := \mathbf{r}^{i+1} - \frac{\langle \mathbf{r}^{i+1}, \mathbf{s}^i \rangle_A}{\langle \mathbf{s}^i, \mathbf{s}^i \rangle_A} \mathbf{s}^i = \mathbf{r}^{i+1} + \frac{(\mathbf{r}^{i+1})^T \mathbf{r}^{i+1}}{(\mathbf{r}^i)^T \mathbf{r}^i} \mathbf{s}^i. \tag{2.4}$$

Now take the inner product with $\mathbf{r}^{i+1}$ on both sides of (2.4) and recall that $(\mathbf{r}^{i+1})^T \mathbf{s}^i = 0$ because $\mathbf{r}^{i+1}$ is orthogonal to L_{i+1} with respect to the standard inner product. Therefore, $(\mathbf{s}^{i+1})^T \mathbf{r}^{i+1} = (\mathbf{r}^{i+1})^T \mathbf{r}^{i+1}$, showing that (2.3) is maintained iteratively. Making the changes from (2.2), (2.3) and (2.4) in steps 2(c), 2(a) and 2(d) respectively, we obtain the final version of the Conjugate Gradient Method. $\square$