15.093 Optimization Methods

Lecture 20: The Conjugate Gradient Algorithm Optimality conditions for constrained optimization

1 Outline

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- 1. The Conjugate Gradient Algorithm
- 2. Necessary Optimality Conditions
- 3. Sufficient Optimality Conditions
- 4. Convex Optimization
- 5. Applications

2 The Conjugate Gradient Algorithm

2.1 Quadratic functions

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$$\min f(\boldsymbol{x}) = \frac{1}{2} \boldsymbol{x'} \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{c'} \boldsymbol{x}$$

<u>Definition:</u> d_1, \ldots, d_n are Q-conjugate if

$$d_i \neq 0, \qquad d'_i Q d_j = 0, \quad i \neq j$$

<u>Proposition:</u> If d_1, \ldots, d_n are <u>Q</u>-conjugate, then d_1, \ldots, d_n are linearly independent.

2.2 Motivation

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Given Q-conjugate d_1, \ldots, d_n , and x^k , compute

$$\begin{aligned} \min_{\alpha} f(\boldsymbol{x}^k + \alpha \boldsymbol{d}_k) &= \boldsymbol{c'} \boldsymbol{x}^k + \alpha \boldsymbol{c'} \boldsymbol{d}_k + \\ \frac{1}{2} (\boldsymbol{x}^k + \alpha \boldsymbol{d}_k)' \boldsymbol{Q} (\boldsymbol{x}^k + \alpha \boldsymbol{d}_k) &= \\ f(\boldsymbol{x}^k) + \alpha \nabla f(\boldsymbol{x}^k)' \boldsymbol{d}_k + \frac{1}{2} \alpha^2 \boldsymbol{d}_k' \boldsymbol{Q} \boldsymbol{d}_k \end{aligned}$$

Solution:

$$\hat{lpha}_k = rac{-
abla f(oldsymbol{x}^k)'oldsymbol{d}_k}{oldsymbol{d}_k'oldsymbol{Q}oldsymbol{d}_k}, \qquad oldsymbol{x}^{k+1} = oldsymbol{x}^k + \hat{lpha}_koldsymbol{d}_k$$

2.3 Expanding Subspace Theorem

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 d_1,\dots,d_n are Q-conjugate. Then, x^{k+1} solves

$$\begin{aligned} & \text{min} \quad f(\boldsymbol{x}) \\ & \text{s.t.} \quad \boldsymbol{x} = \boldsymbol{x}_1 + \sum_{j=1}^k \alpha_j \boldsymbol{d}_j \end{aligned}$$

Moreover, $\boldsymbol{x}^{n+1} = \boldsymbol{x}^*$.

The Algorithm

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Step 0 Given x^1 , set k := 1, $d_1 = -\nabla f(x^0)$

Step 1 For k = 1, ..., n do: If $||\nabla f(\boldsymbol{x}^k)|| \leq \epsilon$, stop; else:

$$\hat{\alpha}_k = \operatorname{argmin}_{\alpha} f(\boldsymbol{x}^k + \alpha \boldsymbol{d}^k) = \frac{-\nabla f(\boldsymbol{x}^k)' \boldsymbol{d}_k}{\boldsymbol{d}_k' \boldsymbol{Q} \boldsymbol{d}_k}$$

$$\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \hat{\alpha}_k \boldsymbol{d}_k$$

$$\begin{aligned} \boldsymbol{x}^{k+1} &= \boldsymbol{x}^k + \hat{\alpha}_k \boldsymbol{d}_k \\ \boldsymbol{d}_{k+1} &= -\nabla f(\boldsymbol{x}^{k+1}) + \lambda_k \boldsymbol{d}_k, \qquad \lambda_k = \frac{-\nabla f(\boldsymbol{x}^{k+1})' \boldsymbol{Q} \boldsymbol{d}_k}{\boldsymbol{d}_k' \boldsymbol{Q} \boldsymbol{d}_k} \end{aligned}$$

2.5Correctness

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Theorem: The directions d_1, \ldots, d_n are Q-conjugate.

2.6 Convergence Properties

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- This is a finite algorithm.
- If there are only k distinct eigenvalues of Q, the CGA finds an optimal solution in k steps.
- Idea of pre-conditioning. Consider

$$\min f(Sx) = \frac{1}{2}(Sx)'Q(Sx) + c'Sx$$

so that the number of distinct eigenvalues of S'QS is small

2.7Example

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$$\mathbf{q} = \begin{pmatrix} 35 & 19 & 22 & 28 & 16 & 3 & 16 & 6 & 4 & 4 \\ 19 & 43 & 33 & 19 & 5 & 2 & 5 & 4 & 0 & 0 \\ 22 & 33 & 40 & 29 & 12 & 7 & 6 & 2 & 2 & 4 \\ 28 & 19 & 29 & 39 & 16 & 7 & 14 & 6 & 2 & 4 \\ 16 & 5 & 12 & 16 & 12 & 4 & 8 & 2 & 4 & 8 \\ 3 & 2 & 7 & 7 & 4 & 5 & 1 & 0 & 1 & 4 \\ 16 & 5 & 6 & 14 & 8 & 1 & 12 & 2 & 2 & 4 \\ 6 & 4 & 2 & 6 & 2 & 0 & 2 & 4 & 0 & 0 \\ 4 & 0 & 2 & 2 & 4 & 1 & 2 & 0 & 2 & 4 \\ 4 & 0 & 4 & 4 & 8 & 4 & 4 & 0 & 4 & 16 \end{pmatrix}$$
 and $\mathbf{c} = \begin{pmatrix} -1 \\ 0 \\ 0 \\ -3 \\ 0 \\ -2 \\ 0 \\ -6 \\ -7 \\ -4 \end{pmatrix}$

 $\kappa(\mathbf{Q}) \approx 17,641$

$$\delta = \left(\frac{\kappa(\mathbf{Q}) - 1}{\kappa(\mathbf{Q}) + 1}\right)^2 = 0.999774 \qquad \text{SLIDE } 9$$

k	$f(\boldsymbol{x}^k)$	$f(\boldsymbol{x}^k) - f(\boldsymbol{x}^*)$	$\frac{f(\boldsymbol{x}^k) - f(\boldsymbol{x}^*)}{f(\boldsymbol{x}^{k-1}) - f(\boldsymbol{x}^*)}$
1	12.000000	2593.726852	1.000000
2	8.758578	2590.485430	0.998750
3	1.869218	2583.596069	0.997341
4	-12.777374	2568.949478	0.994331
5	-30.479483	2551.247369	0.993109
6	-187.804367	2393.922485	0.938334
7	-309.836907	2271.889945	0.949024
8	-408.590428	2173.136424	0.956532
9	-754.887518	1826.839334	0.840646
10	-2567.158421	14.568431	0.007975
11	-2581.711672	0.015180	0.001042
12	-2581.726852	-0.000000	-0.000000

2.8 General problems

Step 0 Given \boldsymbol{x}^1 , set k := 1, $\boldsymbol{d}_1 = -\nabla f(\boldsymbol{x}^0)$

Step 1 If $||\nabla f(\boldsymbol{x}^k)|| \leq \epsilon$, stop; else:

$$\hat{\alpha}_k = \operatorname{argmin}_{\alpha} f(\boldsymbol{x}^k + \alpha \boldsymbol{d}^k) = \frac{-\nabla f(\boldsymbol{x}^k)' \boldsymbol{d}_k}{\boldsymbol{d}_k' Q \boldsymbol{d}_k}$$
$$\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \hat{\alpha}_k \boldsymbol{d}_k$$
$$\boldsymbol{d}_{k+1} = -\nabla f(\boldsymbol{x}^{k+1}) + \lambda_k \boldsymbol{d}_k$$
$$\lambda_k = \frac{||\nabla f(\boldsymbol{x}^{k+1})||}{||\nabla f(\boldsymbol{x}^k)||}$$

Step 2 $k \leftarrow k + 1$, goto Step 1

3 Necessary Optimality Conditions

3.1 Nonlinear Optimization

$$\begin{aligned} & \text{min} \quad f(\boldsymbol{x}) \\ & \text{s.t.} \quad g_j(\boldsymbol{x}) \leq 0, \quad \quad j = 1, \dots, p \\ & \quad h_i(\boldsymbol{x}) = 0, \quad \quad i = 1, \dots, m \end{aligned}$$

$$P = \{ \boldsymbol{x} | g_j(\boldsymbol{x}) \leq 0, \ j = 1, \dots, p, \}$$

 $h_i(\mathbf{x}) = 0, \ i = 1, \dots, m$

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3.2 The KKT conditions

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Discovered by Karush-Kuhn-Tucker in 1950's.

<u>Theorem</u>

If

- \overline{x} is local minimum of P
- $I = \{j | g_i(\overline{x}) = 0\}$, set of tight constraints
- Constraint qualification condition (CQC): The vectors $\nabla g_j(\overline{x}), j \in I$ and $\nabla h_i(\overline{x}), i = 1, \dots, m$, are linearly independent

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Then, there exist vectors (u, v):

1.
$$\nabla f(\overline{x}) + \sum_{j=1}^{p} u_j \nabla g_j(\overline{x}) + \sum_{i=1}^{m} v_i \nabla h_i(\overline{x}) = \mathbf{0}$$

- 2. $u \ge 0$
- 3. $u_j g_j(\overline{x}) = 0, \quad j = 1, \dots, p$

3.3 Some Intuition from LO

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Linearize the functions in the neighborhood of the solution \overline{x} . Problem becomes:

min
$$f(\overline{x}) + \nabla f(\overline{x})'(x - \overline{x})$$

s.t. $g_j(\overline{x}) + \nabla g_j(\overline{x})'(x - \overline{x}) \leq \mathbf{0}, \quad j \in I$
 $h_i(\overline{x}) + \nabla h_i(\overline{x})'(x - \overline{x}) = \mathbf{0}, \quad i = 1, \dots, m$

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This is a LO problem. Dual feasibility:

$$\sum_{j \in I} \hat{u}_j \nabla g_j(\overline{x}) + \sum_{i=1}^m \hat{v}_i \nabla h_i(\overline{x}) = \nabla f(\overline{x}), \quad \hat{u}_j \le 0$$

Change to $u_j = -\hat{u}_j$, $v_i = -\hat{v}_i$ to obtain:

$$\nabla f(\overline{x}) + \sum_{j=1}^{p} u_j \nabla g_j(\overline{x}) + \sum_{i=1}^{m} v_i \nabla h_i(\overline{x}) = \mathbf{0}, \quad u_j \ge 0$$

3.4 Example 1

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min
$$f(\mathbf{x}) = (x_1 - 12)^2 + (x_2 + 6)^2$$

s.t. $h_1(\mathbf{x}) = 8x_1 + 4x_2 - 20 = 0$
 $g_1(\mathbf{x}) = x_1^2 + x_2^2 + 3x_1 - 4.5x_2 - 6.5 \le 0$
 $g_2(\mathbf{x}) = (x_1 - 9)^2 + x_2^2 - 64 \le 0$

$$\overline{\boldsymbol{x}} = (2,1)'; \quad g_1(\overline{\boldsymbol{x}}) = 0, \quad g_2(\overline{\boldsymbol{x}}) = -14, \quad h_1(\overline{\boldsymbol{x}}) = 0.$$

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- $I = \{1\}$
- $\nabla f(\overline{x}) = (-20, 14)'; \nabla g_1(\overline{x}) = (7, -2.5)'$
- $\nabla g_2(\overline{x}) = (-14, 2)'; \nabla h_1(\overline{x}) = (8, 4)'$
- $u_1 = 4$, $u_2 = 0$, $v_1 = -1$
- $\nabla g_1(\overline{x}), \nabla h_1(\overline{x})$ linearly independent
- $\nabla f(\overline{x}) + u_1 \nabla g_1(\overline{x}) + u_2 \nabla g_2(\overline{x}) + v_1 \nabla h_1(\overline{x}) = \mathbf{0}$

$$\begin{pmatrix} -20\\14 \end{pmatrix} + 4 \begin{pmatrix} 7\\-2.5 \end{pmatrix} + 0 \begin{pmatrix} -14\\2 \end{pmatrix} + (-1) \begin{pmatrix} 8\\4 \end{pmatrix} = \begin{pmatrix} 0\\0 \end{pmatrix}$$

3.5 Example 2

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$$\max x'Qx$$

s.t. $x'x \le 1$

Q arbitrary; Not a convex optimization problem.

$$\min \quad -x'Qx$$

s.t.
$$x'x \le 1$$

3.5.1 KKT

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$$-2Qx + 2ux = 0$$

$$x'x \le 1$$

$$u \ge 0$$

$$u(1 - x'x) = 0$$

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3.5.2 Solutions of KKT

- $\overline{x} = 0$, $\overline{u} = 0$, Obj = 0.
- $\overline{x} \neq 0 \Rightarrow Q\overline{x} = \overline{u} \ \overline{x} \Rightarrow \overline{x}$ eigenvector of Q with non-negative eigenvalue \overline{u} .
- $\overline{x}'Q\overline{x} = \overline{u} \ \overline{x}'\overline{x} = \overline{u}$.
- Thus, pick the largest nonnegative eigenvalue \hat{u} of Q. The solution is the corresponding eigenvector \hat{x} normalized such that $\hat{x}'\hat{x} = 1$. If all eigenvalues are negative, $\hat{x} = 0$.

3.6 Are CQC Necessary?

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min
$$x_1$$

s.t. $x_1^2 - x_2 \le 0$
 $x_2 = 0$

Feasible space is (0,0).

KKT:

$$\left(\begin{array}{c} 1\\0 \end{array}\right) + u \left(\begin{array}{c} 2x_1\\-1 \end{array}\right) + v \left(\begin{array}{c} 0\\1 \end{array}\right) = \left(\begin{array}{c} 0\\0 \end{array}\right)$$

KKT multipliers do not exist, while still (0,0)' is local minimum. Check $\nabla g_1(0,0)$ and $\nabla h_1(0,0)$.

3.7 Constrained Qualification

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Slater condition: There exists an x^0 such that $g_j(x^0) < 0$, j = 1, ..., p, and $h_i(x^0) = 0$ for all i = 1, ..., m.

Theorem Under the Slater condition the KKT conditions are necessary.

4 Sufficient Optimality Conditions

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Theorem If

- \overline{x} feasible for P
- Feasible set is P is convex and f(x) convex
- There exist vectors (u, v), $u \ge 0$:

$$\nabla f(\overline{x}) + \sum_{j=1}^{p} u_j \nabla g_j(\overline{x}) + \sum_{i=1}^{m} v_i \nabla h_i(\overline{x}) = \mathbf{0}$$

$$u_j g_j(\overline{\boldsymbol{x}}) = 0, \qquad j = 1, \dots, p$$

Then, \overline{x} is a global minimum of P.

4.1 Proof

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- Let $x \in P$. Then $(1 \lambda)\overline{x} + \lambda x \in P$ for $\lambda \in [0, 1]$.
- $g_j(\overline{x} + \lambda(x \overline{x})) \le 0 \implies$

$$\nabla g_j(\overline{\boldsymbol{x}})'(\boldsymbol{x} - \overline{\boldsymbol{x}}) \le 0$$

• Similarly, $h_i(\overline{x} + \lambda(x - \overline{x})) \leq 0 \Rightarrow$

$$\nabla h_i(\overline{x})'(x-\overline{x}) = 0$$

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• Thus,

$$\nabla f(\overline{x})'(x - \overline{x}) =$$

$$-\left(\sum_{j=1}^{p} u_{j} \nabla g_{j}(\overline{x}) + \sum_{i=1}^{m} v_{i} \nabla h_{i}(\overline{x})\right)'(x - \overline{x}) \ge 0$$

$$\Rightarrow f(x) \ge f(\overline{x}).$$

5 Convex Optimization

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- The KKT conditions are always necessary under CQC.
- The KKT conditions are sufficient for convex optimization problems.
- The KKT conditions are necessary and sufficient for convex optimization problems under CQC.
- $\min f(x)$ s.t. Ax = b, $x \ge 0$, f(x) convex, KKT are necessary and sufficient even without CQC.

5.0.1 Separating hyperplanes

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Theorem Let S be a nonempty closed convex subset of \Re^n and let $\boldsymbol{x}^* \in \Re^n$ be a vector that does not belong to S. Then, there exists some vector $\boldsymbol{c} \in \Re^n$ such that $\boldsymbol{c}'\boldsymbol{x}^* < \boldsymbol{c}'\boldsymbol{x}$ for all $\boldsymbol{x} \in S$.

Proof in BT, p.170

5.1 Sketch of the Proof under convexity

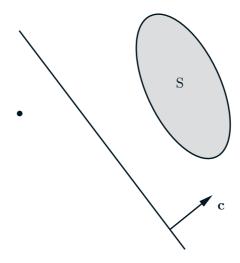
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- Suppose \overline{x} is a local (and thus global) optimal solution.
- $f(x) < f(\overline{x}), g_j(x) \le 0, j = 1, ..., p, h_i(x) = 0, i = 1, ..., m$ is infeasible.
- Let $U = \{(u_0, u, v) | \text{ there exists } x : f(x) < u_0, g_j(x) \le u_j, h_i(x) = v_i \}.$
- $(f(\overline{x}), \mathbf{0}, \mathbf{0}) \notin S$.
- ullet U convex.

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• By separating hyperplane theorem, there is a vector (c_0, c, d) :

$$c_0 u_0 + \sum_{j=1}^p c_j u_j + \sum_{i=1}^m d_i v_i > c_0 f(\overline{\boldsymbol{x}}) \ \forall \ (u_0, \boldsymbol{u}, \boldsymbol{v}) \in U.$$



• $c_0 \ge 0$ and $c_j \ge 0$ for $j \in I$ (constraint $g_j(\overline{x}) \le 0$ tight). Why? If $(u_0, \boldsymbol{u}, \boldsymbol{v}) \in U$, then $(u_0 + \lambda, \boldsymbol{u}, \boldsymbol{v}) \in U$ for $\lambda \ge 0$. Thus,

$$\forall \lambda \geq 0, \ \lambda c_0 + \sum_{j=1}^p c_j u_j + \sum_{i=1}^m d_i v_i > c_0 f(\overline{x}) \ \Rightarrow \ c_0 \geq 0.$$

• Select $(u_0, u, v) = (f(x) + \lambda, g_1(x), \dots, g_p(x), h_1(x), \dots, h_m(x)) \in U$

• $c_0(f(\boldsymbol{x}) + \lambda) + \sum_{i=1}^p c_j g_j(\boldsymbol{x}) + \sum_{i=1}^m d_i h_i(\boldsymbol{x}) > c_0 f(\overline{\boldsymbol{x}})$

• Take $\lambda \to 0$:

$$c_0f(oldsymbol{x}) + \sum_{j=1}^p c_jg_j(oldsymbol{x}) + \sum_{i=1}^m d_ih_i(oldsymbol{x}) \geq c_0f(\overline{oldsymbol{x}})$$

• $c_0 > 0$ (constrained qualification needed here).

 $f(\boldsymbol{x}) + \sum_{j=1}^{p} u_j g_j(\boldsymbol{x}) + \sum_{i=1}^{m} v_i h_i(\boldsymbol{x}) \ge f(\overline{\boldsymbol{x}}), \quad u_j \ge 0$

 $f(\overline{x}) + \sum_{j=1}^{p} u_j g_j(\overline{x}) + \sum_{i=1}^{m} v_i h_i(\overline{x}) \le f(\overline{x}) \le \frac{1}{p}$

$$f(x) + \sum_{j=1}^{p} u_j g_j(x) + \sum_{i=1}^{m} v_i h_i(x).$$

• Thus,

$$f(\overline{x}) = \min \left(f(x) + \sum_{j=1}^{p} u_j g_j(x) + \sum_{i=1}^{m} v_i h_i(x) \right)$$
$$\sum_{j=1}^{p} u_j g_j(\overline{x}) = 0 \quad \Rightarrow \quad u_j g_j(\overline{x}) = 0$$

• Unconstrained optimality conditions:

$$\nabla f(\overline{x}) + \sum_{j=1}^{p} u_j \nabla g_j(\overline{x}) + \sum_{i=1}^{m} v_i \nabla h_i(\overline{x}) = \mathbf{0}$$

6 Applications

6.1 Linear Optimization

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s.t.
$$Ax = b$$
 $x \ge 0$
min $c'x$
s.t. $Ax - b = 0$
 $-x \le 0$

 $\min c'x$

6.1.1 KKT

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$$egin{array}{lll} c + A' \hat{u} - v & = & \mathbf{0} \\ v & \geq & \mathbf{0} \\ v_j x_j & = & 0 \\ Ax - b & = & \mathbf{0} \\ x & \geq & \mathbf{0} \end{array}$$

 $u=-\hat{u}$

$$egin{array}{lll} m{A'u} & \leq & m{c} & ext{dual feasibility} \ (c_j - m{A'_j u}) x_j & = & 0 & ext{complementarity} \ m{Ax - b} & = & m{0} & ext{primal feasibility} \ m{x} & \geq & m{0} & ext{primal feasibility} \end{array}$$

6.2 Portfolio Optimization

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 \boldsymbol{x} =weights of the portfolio

$$\max_{\text{s.t.}} \quad \boldsymbol{r'x} - \lambda \frac{1}{2} \boldsymbol{x'Qx}$$
 s.t.
$$\boldsymbol{e'x} = 1$$

$$\min_{\text{s.t.}} \quad -\boldsymbol{r'x} + \lambda \frac{1}{2} \boldsymbol{x'Qx}$$
 s.t.
$$\boldsymbol{e'x} = 1$$

6.2.1 KKT

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$$-r + \lambda Qx + ue = 0$$

$$x = \frac{1}{\lambda}Q^{-1}(r - ue)$$

$$e'x = 1 \Rightarrow e'Q^{-1}(r - ue) = \lambda$$

$$u = \frac{e'Q^{-1}r - \lambda}{e'Q^{-1}e}$$

As λ changes, tradeoff of risk and return changes. The allocation changes as well. This is the essense of modern portfolio theory.

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