236330 - Introduction to Optimization: Homework #4

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Amit Rotner
123456789
Or Steiner
123456789

DNNs, Augmented Lagrangian and Constrained Optimization

Part 1 – Deep Neural Network:

Task 1:

$$f\left(x_1, x_2\right) = x_1 e^{-\left(x_1^2+x_1^2\right)} \ , \phi = tanh\left(x\right) = \frac{1-e^x}{1+e^x}$$

$$\langle A, B\rangle = Tr\left(A^T B\right) = Tr\left(AB^T\right)$$

$$F\left(x, W_1, W_2, W_3, b_1, b_2, b_3\right) = W_3^T \phi_2\left(W_2^T \phi_1\left(W_1^T x + b_1\right) + b_2\right) + b_3$$

$$r_i = F\left(x^i, W\right) - y_i$$

$$\psi\left(r\right) = r^2$$

$$\nabla_r \psi = 2r$$

$$E = \psi(r)$$

$$\nabla_x E = J_{F(x)}^T \nabla_r \psi$$

$$J_{F(x)} = W_3^T \Phi_2' W_2^T \Phi_1' W_1^T$$

Let us denote$u_1 = W_1^T x + b_1$ and $du_1 = dW_1^T x$.

$$dE = \nabla_{u_1} E^T du_1 = \nabla_{u_1} E^T dW_1^T x = Tr\left(\nabla_{u_1} E^T dW_1^T x\right) = Tr\left(x \nabla_{u_1} E^T dW_1^T\right) = \left\langle x \nabla_{u_1} E^T, dW_1\right\rangle$$

$$\nabla_{u_1} E = \Phi_1' W_2 \Phi_2' W_3 \nabla_r \psi$$

And therefore the gradient of the Error with respect to W_1 is:

$$\nabla_{W_1} E = x \nabla_r \psi W_3^T \Phi_2' W_2^T \Phi_1'$$

Let us denote $u_1 = W_1^T x + b_1$ and $du_1 = db_1$.

$$dE = \nabla_{u_1} E^T du_1 = \nabla_{u_1} E^T db_1 = Tr\left(\nabla_{u_1} E^T db_1\right) = \langle \nabla_{u_1} E, db_1 \rangle$$

$$\nabla_{u_1} E = \Phi_1' W_2 \Phi_2' W_3 \nabla_r \psi$$

And therefore the gradient of the Error with respect to b_1 is:

$$\nabla_{b_1} E = \Phi_1' W_2 \Phi_2' W_3 \nabla_r \psi$$

Let us denote $u_2 = W_2^T \phi_1\left(W_1^T x + b_1\right) + b_2$ and $du_2 = dW_2^T \phi_1(u_1)$.

$$dE = \nabla_{u_2} E^T du_2 = \nabla_{u_2} E^T dW_2^T \phi_1(u_1) = Tr\left(\nabla_{u_2} E^T dW_2^T \phi_1(u_1)\right) = Tr\left(\phi_1(u_1) \nabla_{u_2} E^T dW_2^T\right) = \left\langle \phi_1 u_1 \nabla_{u_2} E^T, dW_2 \right\rangle$$

$$\nabla_{u_2} E = \Phi_2' W_3 \nabla_r \psi$$

And therefore the gradient of the Error with respect to W_2 is:

$$\nabla_{W_2} E = \phi_1(u_1) \nabla_r \psi W_3^T \Phi_2'$$

Let us denote $u_2 = W_2^T \phi_1\left(W_1^T x + b_1\right) + b_2$ and $du_2 = db_2$.

$$dE = \nabla_{u_2} E^T du_2 = \nabla_{u_2} E^T db_2 = Tr\left(\nabla_{u_2} E^T db_2\right) = Tr\left(\nabla_{u_2} E^T db_2\right) = \langle \nabla_{u_2} E, db_2 \rangle$$

$$\nabla_{u_2} E = \Phi_2' W_3 \nabla_r \psi$$

And therefore the gradient of the Error with respect to b_2 is:

$$\nabla_{b_2} E = \Phi_2' W_3 \nabla_r \psi$$

Let us denote $u_3 = W_3^T \phi_2\left(W_2^T \phi_1\left(W_1^T x + b_1\right) + b_2\right) + b_3$ and $du_3 = dW_3^T \phi_2(u_2)$.

$$dE = \nabla_{u_3} E^T du_3 = \nabla_{u_3} E^T dW_3^T \phi_2(u_2) = Tr\left(\nabla_{u_2} E^T dW_3^T \phi_2(u_2)\right) = Tr\left(\phi_2(u_2) \nabla_{u_3} E^T dW_3^T\right) = \left\langle \phi_2 u_2 \nabla_{u_3} E^T, dW_3 \right\rangle$$

$$\nabla_{u_3} E = \nabla_r \psi$$

And therefore the gradient of the Error with respect to W_3 is:

$$\nabla_{W_3} E = \phi_2 \left(u_2\right) \nabla_r \psi$$

Let us denote$u_3 = W_3^T \phi_2 \left(W_2^T \phi_1 \left(W_1^T x + b_1\right) + b_2\right) + b_3$ and $du_3 = db_3$.

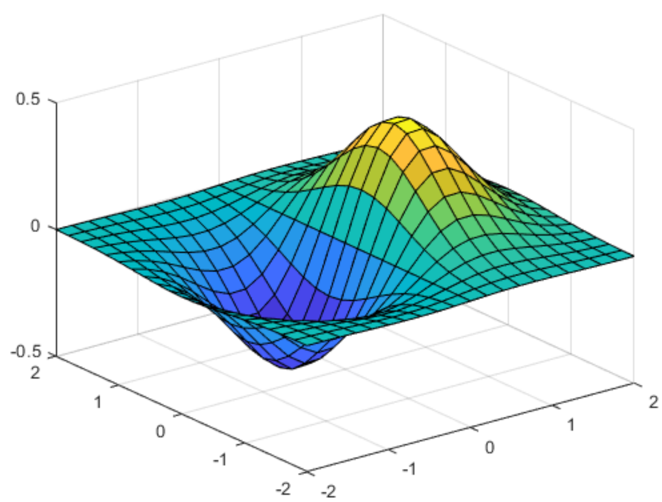
$$dE = \nabla_{u_3} E^T du_3 = \nabla_{u_3} E^T db_3 = Tr\left(\nabla_{u_2} E^T db_3\right) = Tr\left(\nabla_{u_3} E^T db_3\right) = \langle \nabla_{u_3} E, db_3 \rangle$$

$$\nabla_{u_3} E = \nabla_r \psi$$

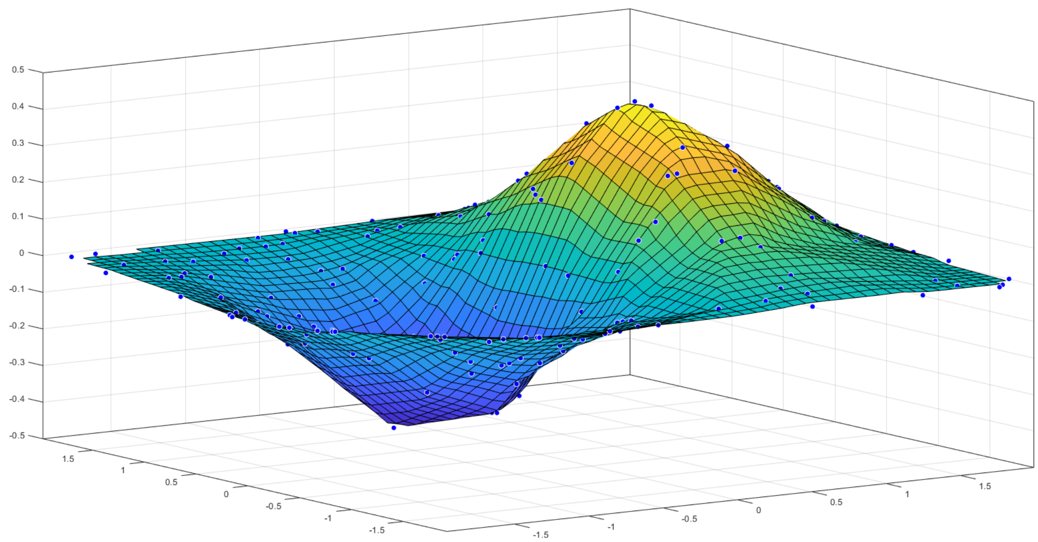
And therefore the gradient of the Error with respect to b_3 is:

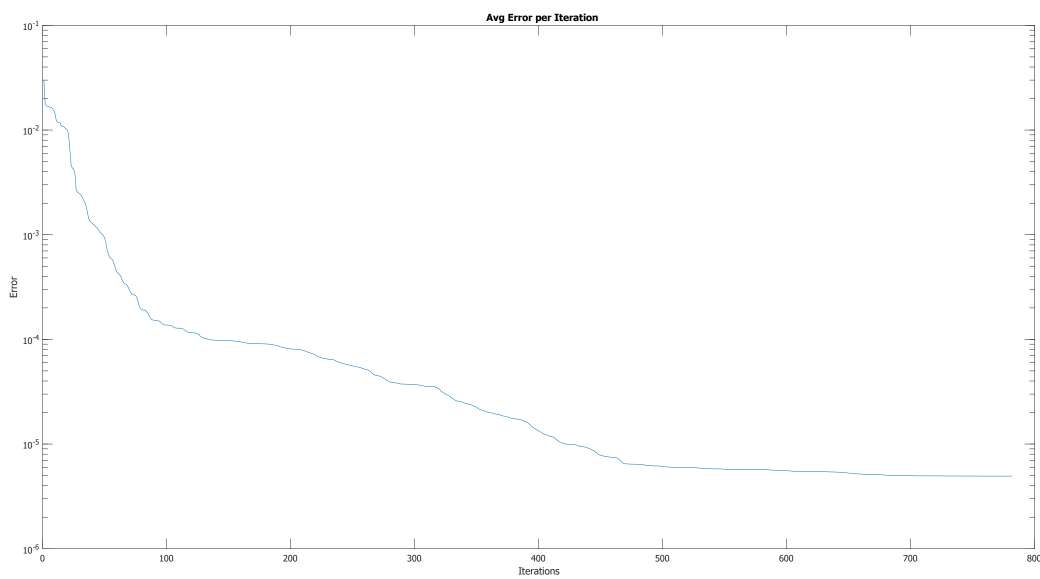
$$\nabla_{b_3} E = \nabla_r \psi$$

Task 2: Plotting the Objective Function yields:



Task 3: Plotting the network reconstruction yields:





Part 2 – Augmented Lagrangian:

Task 1: Consider the following quadratic problem:

$$\min_x 2\left(x_1-5\right)^2+\left(x_2-1\right)^2$$

s.t.

$$
\begin{aligned}
x_2 \leq& 1 - \frac{x_1}{2} \\
x_2 \geq& x_1 \\
x_2 \geq& -x_1
\end{aligned}
$$

1. Is this problem convex?
2. Find the optimal solution (x^*, λ^*)
3. Calculate the Lagrange multipliers using KKT conditions. What is the optimal value of the objective function?

Solution:

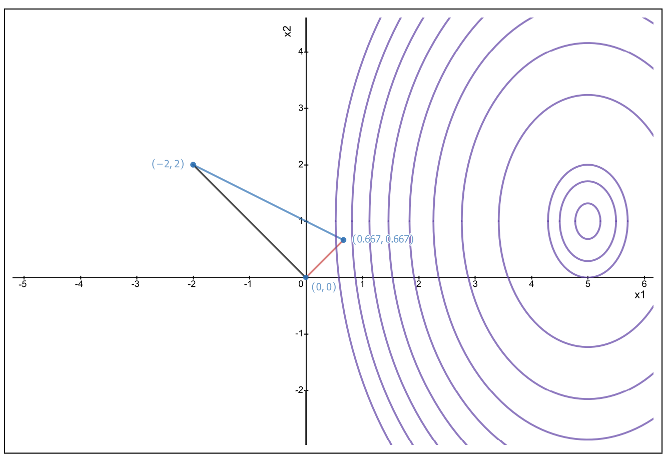


Figure 1: The feasible area and the level sets of the objective function

1. Therefore the active constraints are c_1 and c_2.
2. It is fairly clear from the figure above that the solution is $x^* = \left(\frac{2}{3}, \frac{2}{3}\right)^T$.
3. Writing the Lagrangian yields:

$$\mathcal{L}(x, \lambda) = 2(x_1 - 5)^2 + (x_2 - 1)^2 + \lambda_1 \left(x_2 - 1 + \frac{x_1}{2}\right) + \lambda_2 (x_1 - x_2) + \lambda_3 (-x_1 - x_2)$$

First we find the gradient of the Lagrangian:

$$\nabla_x \mathcal{L}(x, \lambda) = \left(4(x_1 - 5) + 0.5\lambda_1 + \lambda_2 - \lambda_3, \quad 2(x_2 - 1) + \lambda_1 - \lambda_2 - \lambda_3\right)$$

If x^* is an optimal solution for our problem, then there exist λ^* which satisfies the KKT conditions:

(a) $\nabla_{x_1} \mathcal{L}(x^*, \lambda) = 0 \Rightarrow 4(x_1 - 5) + 0.5\lambda_1 + \lambda_2 - \lambda_3 = 0$

(b) $\nabla_{x_2}\mathcal{L}(x^*,\lambda)=0 \Rightarrow 2(x_2-1)+\lambda_1-\lambda_2-\lambda_3=0$

(c) $x_2-1+\frac{x_1}{2}\leq 0$

(d) $x_1-x_2\leq 0 \Rightarrow x_1\leq x_2$

(e) $-x_1-x_2\leq 0 \Rightarrow -x_2\leq x_1$

(f) $\lambda^*\geq 0$

(g) $\lambda_1\left(x_2-1+\frac{x_1}{2}\right)=0$

(h) $\lambda_2(x_1-x_2)=0$

(i) $\lambda_3(-x_1-x_2)=0$

From (9) we get:

$$\lambda_3=0$$

From $(1)+(2)$ we get:

$$0.5\lambda_1+\lambda_2=17\frac{1}{3}$$
$$\lambda_1-\lambda_2=\frac{2}{3}$$

Therefore, we get $\lambda_1=12, \lambda_2=11\frac{1}{3}$.

In conclusion:

$$x^*=\left(\frac{2}{3},\frac{2}{3}\right)^T,\ \lambda^*=\left(12,11\frac{1}{3},0\right)^T$$

Hence, the optimal value of the objective function is:

$$2\left(\frac{2}{3}-5\right)^2+\left(\frac{2}{3}-1\right)^2=37\frac{2}{3}$$

4. From the above, we know that:

$$\mathcal{L}(x,\lambda)=2(x_1-5)^2+(x_2-1)^2+\lambda_1\left(x_2-1+\frac{x_1}{2}\right)+\lambda_2(x_1-x_2)+\lambda_3(-x_1-x_2)$$

If we hold $\lambda_1,\lambda_2,\lambda_3$ fixed, this is a convex function of $(x_1,x_2)^T$.

Therefore, the infimum with respect to $(x_1,x_2)^T$ is achieved when the partial derivatives with respect to x_1 and x_2 are zero, that is,

$$4(x_1-5)+0.5\lambda_1+\lambda_2-\lambda_3=0$$

$$2(x_2-1)+\lambda_1-\lambda_2-\lambda_3=0$$

Hence,

$$x_1=\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{4}$$

$$x_2 = \frac{2-\lambda_1+\lambda_2+\lambda_3}{2}$$

By substituting these infimal values into $\mathcal{L}(x,\lambda)$ we obtain the dual objective:

$$\begin{aligned}
\mathcal{L}(x,\lambda) &= 2(x_1-5)^2+(x_2-1)^2+\lambda_1\left(x_2-1+\frac{x_1}{2}\right)+\lambda_2(x_1-x_2)+\lambda_3(-x_1-x_2)\\
&= 2\left(\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{4}-5\right)^2+\left(\frac{2-\lambda_1+\lambda_2+\lambda_3}{2}-1\right)^2\\
&+\lambda_1\left(\frac{2-\lambda_1+\lambda_2+\lambda_3}{2}-1+\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{8}\right)+\lambda_2\left(\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{4}-\frac{2-\lambda_1+\lambda_2+\lambda_3}{2}\right)\\
&+\lambda_3\left(-\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{4}-\frac{2-\lambda_1+\lambda_2+\lambda_3}{2}\right)
\end{aligned}$$

5. Hence, the dual problem is:

$$\begin{aligned}
\max_{\lambda\geq 0} 2&\left(\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{4}-5\right)^2+\left(\frac{2-\lambda_1+\lambda_2+\lambda_3}{2}-1\right)^2\\
&+\lambda_1\left(\frac{2-\lambda_1+\lambda_2+\lambda_3}{2}-1+\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{8}\right)+\lambda_2\left(\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{4}-\frac{2-\lambda_1+\lambda_2+\lambda_3}{2}\right)\\
&+\lambda_3\left(-\frac{20-0.5\lambda_1-\lambda_2+\lambda_3}{4}-\frac{2-\lambda_1+\lambda_2+\lambda_3}{2}\right)
\end{aligned}$$

6. Substitute the Lagrange multipliers from section 3 into the dual problem, yields that the value of the dual problem is $= 37\frac{2}{3}$ which it also the optimum of the dual problem.
Since it is also the optimal value of the primal problem, the duality gap is zero.

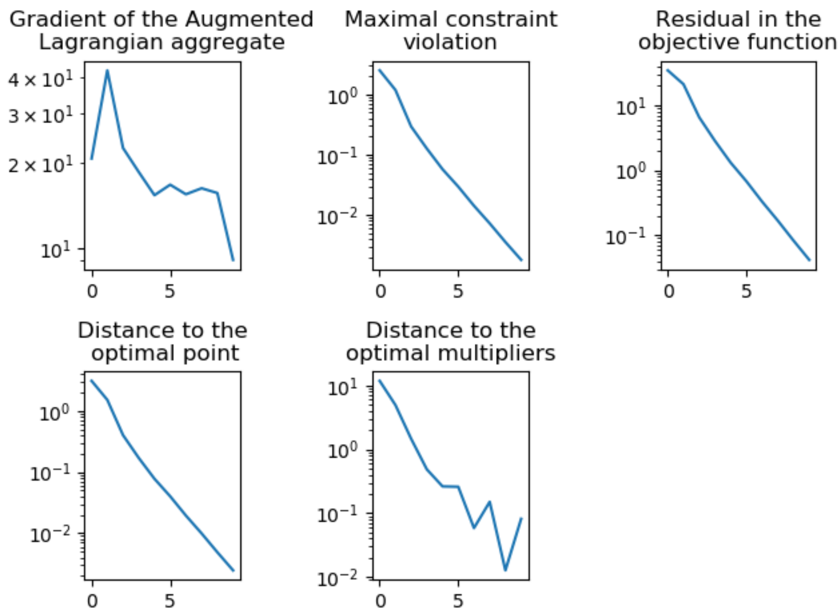
Task 2: Writing the quadratic programming problem used in Task 1 in general form, yields:

$$\frac{1}{2}\begin{pmatrix} x_1 & x_2 \end{pmatrix}\underbrace{\begin{pmatrix} 4 & 0 \\ 0 & 2 \end{pmatrix}}_{Q}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}+\underbrace{\begin{pmatrix} -20 & -2 \end{pmatrix}}_{d^T}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}+\underbrace{51}_{e}$$

s.t.

$$\underbrace{\begin{pmatrix} 0.5 & 1 \\ 1 & -1 \\ -1 & -1 \end{pmatrix}}_{A}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}-\underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}_{b}\leq 0$$

Using the Augmented Lagrangian Solver to Solve a Quadratic Programming Problem:



Part 3 – Constrained Optimization:

Task 1: Consider the following optimization problem:

$$\min_{x} x^T M x + c^T x$$

s.t.

$$Ax = b$$
$$M \succ 0$$
$$A \in \mathbb{R}^{m \times n}, x \in \mathbb{R}^n, c \in \mathbb{R}^n, b \in \mathbb{R}^n, M \in \mathbb{R}^{m \times m}$$

1. Is this problem convex?
2. Find the optimal solution (x^*, λ^*)

Solution:

1. We start by finding the Hessian of the objective function:

$$\begin{aligned} df &= dx^T Mx + x^T M dx + c^T dx \\ &= x^T M^T dx + x^T M dx + c^T dx \\ &\underset{(i)}{=} 2x^T M dx + c^T dx \\ &\underset{(ii)}{=} \left(2x^T M + c^T\right) dx \\ &= (2Mx + c)^T dx \end{aligned}$$

(i) - Since $dx^T Mx$ is a scalar.

(ii) - Since $M = M^T$.

And therefore: $\nabla f = 2Mx + c$

Now,

$$d\nabla f = 2M dx$$

Hence, $H = 2M$.

We know that $M \succ 0$ and therefore $H = 2M$ is also PD and the problem is convex.

2. Writing the Lagrangian yields:

$$\mathcal{L}(x, \lambda) = f(x) + \lambda (Ax - b)$$

First we find the gradient of the Lagrangian:

$$\nabla_x \mathcal{L}(x, \lambda) = 2Mx + c + \lambda A^T$$

If x^* is an optimal solution for our problem, then there exist λ^* which satisfies the KKT conditions:

(a) $\nabla_x \mathcal{L}(x, \lambda) = 0 \Rightarrow 2Mx^* + \lambda A^T = -c$

(b) $Ax^* - b = 0$

Writing the above as a linear system:

$$\begin{pmatrix} 2M & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} x^* \\ \lambda^* \end{pmatrix} = \begin{pmatrix} -c \\ b \end{pmatrix}$$

Assuming A is invertible and since M is PD, then $\begin{pmatrix} 2M & A^T \\ A & 0 \end{pmatrix}$ is also invertible and:

$$\begin{pmatrix} x^* \\ \lambda^* \end{pmatrix} = \begin{pmatrix} 2M & A^T \\ A & 0 \end{pmatrix}^{-1} \begin{pmatrix} -c \\ b \end{pmatrix}$$

Task 2: Consider the following optimization problem:

$$\underset{x}{min}\ \|x-c\|_2^2$$

s.t.

$$Ax=b$$
$$A\in\mathbb{R}^{m\times n}, x\in\mathbb{R}^n, c\in\mathbb{R}^n, b\in\mathbb{R}^n$$

1. Is this problem convex?
2. Find the optimal solution (x^*,λ^*)

Solution:

1. We start by proving that the objective function is convex:

   We have seen in class that the Euclidean norm $\|\cdot\|_2$ is convex and therefore $h(x)=\|x-c\|_2$ is also convex.

   Since $g(x)=x^2$ is convex as well, and also it is non-decreasing on $[0,\infty)$, the range of h, the composition $f=f\circ h=\|x-c\|_2^2$ is convex.

   Hence, the problem is convex.

2. Writing the Lagrangian yields:

   $$\mathcal{L}(x,\lambda)=f(x)+\lambda(Ax-b)$$

   First we find the gradient of the Lagrangian:

   $$\nabla_x\mathcal{L}(x,\lambda)=2x^Tx-2x^Tc+\lambda A^T$$

   If x^* is an optimal solution for our problem, then there exist λ^* which satisfies the KKT conditions:

   (a) $\nabla_x\mathcal{L}(x,\lambda)=0\Rightarrow 2x^{*T}x^*-2x^{*T}c=\lambda A^T$

   (b) $Ax^*-b=0$

   Assuming A is invertible, then $x^*=A^{-1}b$.

   Hence,

   $$2b^T\left(A^{-1}\right)^TA^{-1}b-2b^T\left(A^{-1}\right)^Tc=\lambda A^T$$

   $$\lambda^*=2b^T\left(AA^T\right)^{-1}b\left(A^T\right)^{-1}-2b^T\left(A^{-1}\right)^Tc\left(A^T\right)^{-1}$$

   Therefore, the optimal solution is:

   $$(x^*,\lambda^*)=\left(A^{-1}b,2b^T\left(AA^T\right)^{-1}b\left(A^T\right)^{-1}-2b^T\left(A^{-1}\right)^Tc\left(A^T\right)^{-1}\right)$$