TMA4180 Optimization 1
Project 2: Constrained Optimization

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Introduction

Constrained optimization problems can be handled in several ways. In this report we first derive sufficient and necessary conditions for optimality, and then evaluate our implementation on various test cases.

Question 1

To show that the problem of minimizing $\hat{f}(A,b) = \sum_{i=1}^{m} \hat{r}_i(A,b)^2$ is convex, where the eigenvalues of A are restricted as in the following equations

$$0 \geq \underline{\lambda} - \lambda_{min}(A) = \underline{\lambda} - \text{min } x^T Ax = \hat{c}_1, \qquad \text{with } \|x\|_2 = 1 \tag{1}$$

$$0 \geq \lambda_{max}(A) - \overline{\lambda} = \text{max } x^T Ax - \overline{\lambda} = \hat{c}_2, \qquad \text{with } \|x\|_2 = 1 \tag{2}$$

we need to show that the objective function is convex and that the domain of $\hat{f}$ with constraints, i.e. the feasible set is convex. From project 1, we showed that min $\hat{f}(x)$ was convex by using the properties of the function being a composition of an affine and a convex function. Our feasible set S is where (1) and (2) are fulfilled, and S=U $\cap$ V, where U and V are defined as below

$$U := \text{all x when } \hat{c}_1(x) \leq 0 \iff \hat{c}_1^{-1}(-\infty, 0] \tag{3}$$

$$V := \text{all x when } \hat{c}_2(x) \leq 0 \iff \hat{c}_2^{-1}(-\infty, 0]. \tag{4}$$

To show that S is convex, we need U and V to be convex sets. For set U: For B_1, B_2 in U, we need that the linear combination $tB_1 + (1-t)B_2$ also is in U, which means that (1) is fulfilled. Using the relation $-\text{min } (r+s) \leq -\text{min } (r) - \text{min } (s)$ and inserting the inequality min $x^T Ax \geq \underline{\lambda}$

$$\begin{aligned} \underline{\lambda} - \text{min } x^T(tB_1 + (1-t)B_2)x &= \underline{\lambda} - \text{min } (tx^T B_1 x + (1-t)x^T B_2 x) \\ &\leq \underline{\lambda} - t\text{min } x^T B_1 x - (1-t)\text{min } x^T B_2 x \\ &\leq \underline{\lambda} - t\underline{\lambda} - (1-t)\underline{\lambda} \\ &= 0 \end{aligned} \tag{5}$$

Since $\underline{\lambda} - \text{min } x^T(tB_1 + (1-t)B_2)x$ is less than 0, $tB_1 + (1-t)B_2$ is in U, and the set U is convex.

For V: For D_1, D_2 in V, we need that the linear combination $tD_1 + (1-t)D_2$ also is in V, which means that (2) is fulfilled. Using the relation max $(r+s) \leq$ max (r) + max (s) and inserting the inequality max $x^T Ax \leq \overline{\lambda}$

$$\begin{aligned} \text{max } x^T(tD_1 + (1-t)D_2x - \overline{\lambda} &= \text{max}(tx^T D_1 x + (1-t)x^T D_2 x) - \overline{\lambda} \\ &\leq t\text{max } x^T D_1 x + (1-t)\text{max } x^T D_2 x - \overline{\lambda} \\ &\leq t\overline{\lambda} + (1-t)\overline{\lambda} - \overline{\lambda} \\ &= 0 \end{aligned} \tag{6}$$

Since max $x^T(tD_1 + (1-t)D_2)x - \overline{\lambda}$ is less than 0, $tD_1 + (1-t)D_2$ is in V, and the set V is convex. The intersection of two convex sets is convex, and thus, S = U ∩ V is convex. We have then showed that the problem defined is convex.

Question 2

Let's rewrite $\hat{f}(A_{11}, A_{22}, A_{12}) = \hat{f}(x, y, z) = (xy)^{1/2} - (\underline{\lambda}^2 + z^2)^{1/2}$. We first observe that $\hat{f}(x, y, z)$ is real on the set $\{x, y, z \in \mathbb{R}^3 | x > 0, y > 0\}$, since $xy > 0$ and $(\underline{\lambda}^2 + z^2)^{1/2} > 0$. Since the first and second derivatives of these functions will have no singularities for $x > 0, y > 0$, they will obviously be continuous. Thus the function is twice continuously differentiable.

To show that the function is concave, we need that the Hessian, $H = D^2(\hat{f}(x, y, z))$ is negative semi-definite, i.e.

$$\boldsymbol{u}^T H \boldsymbol{u} \leq 0, \tag{7}$$

for $\boldsymbol{u} = [u_1, u_2, u_3]^T \in \mathbb{R}^n$. The derivative and the Hessian of f(x,y,z) is given by:

$$D(f(x,y,z)) = \Big[\frac{y}{2\sqrt{xy}}, \frac{x}{2\sqrt{xy}}, -\frac{z}{\sqrt{\underline{\lambda}^2 + z^2}}\Big] \tag{8}$$

$$H = \begin{bmatrix} -y^2\beta & \xi - xy\beta & 0 \\ \xi - xy\beta & -x^2\beta & 0 \\ 0 & 0 & -(\underline{\lambda}^2 + z^2)^{-\frac{1}{2}} + z^2(\underline{\lambda}^2 + z^2)^{-\frac{3}{2}} \end{bmatrix}, \tag{9}$$

where $\xi = \frac{1}{2}(xy)^{-1/2}$ and $\beta = \frac{1}{4}(xy)^{-3/2}$. Inserting into (7) and multiplying by -1, we get

$$\beta y^2 u_1^2 - \xi u_1 u_2 + \beta x^2 u_2^2 + (\underline{\lambda}^2 + z^2)^{-1/2}(1 - \frac{z^2}{\underline{\lambda}^2 + z^2})u_3^2 \geq 0 \tag{10}$$

Dividing by βy^2, and write as square, we get

$$(u_1 - \frac{x}{y}u_2)^2 + (\underline{\lambda}^2 + z^2)^{-1/2}(1 - \frac{z^2}{\underline{\lambda}^2 + z^2})u_3^2 \geq 0. \tag{11}$$

The inequality holds since $x > 0, y > 0$, and we can conclude that the Hessian is negative semi-definite, and thus the function is concave.

Question 3

The constraints given in the project are:

$$\underline{\lambda} \leq A_{11} \leq \overline{\lambda} \qquad \Leftrightarrow \qquad \underline{\lambda} \leq x_1 \leq \overline{\lambda} \tag{12}$$

$$\underline{\lambda} \leq A_{22} \leq \overline{\lambda} \qquad \Leftrightarrow \qquad \underline{\lambda} \leq x_3 \leq \overline{\lambda} \tag{13}$$

$$(A_{11}A_{22})^{1/2} \geq (\underline{\lambda}^2 + A_{12}^2)^{1/2} \qquad \Leftrightarrow \qquad (x_1x_3)^{1/2} \geq (\underline{\lambda}^2 + x_2^2)^{1/2} \tag{14}$$

(12) is equivalent to the union of the following constraints.

$$c_1 = x_1 - \underline{\lambda} \geq 0 \tag{15}$$

$$c_2 = -x_1 + \overline{\lambda} \geq 0 \tag{16}$$

Similarly, (13) is equivalent to the following two.

$$c_3 = x_3 - \underline{\lambda} \geq 0 \tag{17}$$

$$c_4 = -x_3 + \overline{\lambda} \geq 0 \tag{18}$$

We could keep (14) as it is, or equivalently take its square.

$$c_5 = x_1x_3 \geq \underline{\lambda}^2 + x_2^2 \qquad \Leftrightarrow \qquad x_1x_3 - \underline{\lambda}^2 - x_2^2 \geq 0 \tag{19}$$

We now have five inequality constraints and no equality constraints:

$$c_1(x) = x_1 - \underline{\lambda} \geq 0 \tag{20}$$
$$c_2(x) = -x_1 + \overline{\lambda} \geq 0. \tag{21}$$
$$c_3(x) = x_3 - \underline{\lambda} \geq 0 \tag{22}$$
$$c_4(x) = -x_3 + \overline{\lambda} \geq 0 \tag{23}$$
$$c_5(x) = x_1 x_3 - \underline{\lambda}^2 - x_2^2 \geq 0 \tag{24}$$

Slater's constraint qualification

Slater's constraint qualification holds when the constraints c_i are concave for all $i \in \mathcal{I}$, linear for all $i \in \mathcal{E}$, and there is a feasible point $\hat{x}$ such that $c_i(\hat{x}) > 0$, for all $i \in \mathcal{I}$. Concave c_i is equivalent to convex $-c_i$. We want to show that:

$$-c_i(\lambda x_a + (1-\lambda)x_b) \leq \lambda(-c_i(x_a)) + (1-\lambda)(-c_i(x_b)) \tag{25}$$

for all x_a, $x_b \in \mathbb{R}^5$, for all $\lambda \in [0,1]$, for all $i \in \{1,2,3,4,5\}$.

The first four constraints are linear in all elements of x, and consequently concave.

$$-c_5 = \underline{\lambda}^2 + x_2^2 - x_1 x_3, \tag{26}$$

$-c_5$ is linear in x_1 and x_3, and therefore also convex in these variables, making c_5 concave in them. Now to x_2. Inserting (26) into (25) and cancelling the $\underline{\lambda}^2$ and $-x_1x_3$ terms which are independent of x_2, we want to show that the x_2^2 term is convex:

$$(\lambda x_{2a} + (1-\lambda)x_{2b})^2 \leq \lambda x_{2a}^2 + (1-\lambda)x_{2b}^2$$

This is identical to the proof in project 1. Since $-c_i$ is convex in x_2, c_i is concave in x_2. We have now shown that all the constraint functions are concave. It remains to show that there exists a feasible point $\hat{x}$ such that $c_i(\hat{x}) > 0$, for all $i \in \mathcal{I}$.

Now if we choose $x_1' = x_3' = (\underline{\lambda} + \overline{\lambda})/2$, then by simple inspection, $c_i > 0, i \in [1,2,3,4]$. Then let $x_2' = \sqrt{(x_1'x_3' - \underline{\lambda}^2)/2}$. Inserted into c_5 this yields

$$c_5(x') = x_1'x_3' - \underline{\lambda}^2 - \left(\sqrt{\frac{x_1'x_3' - \underline{\lambda}^2}{2}}\right)^2 = \frac{x_1'x_3' - \underline{\lambda}^2}{2} = \frac{(\frac{\underline{\lambda}+\overline{\lambda}}{2})^2 - \underline{\lambda}^2}{2} = \frac{\overline{\lambda}^2 + 2\underline{\lambda}\overline{\lambda} - 3\underline{\lambda}^2}{8} > 0 \tag{27}$$

Since $\overline{\lambda}$ is strictly larger than $\underline{\lambda}$, both $\overline{\lambda}^2$ and $\overline{\lambda}\underline{\lambda}$ must be strictly larger than $\underline{\lambda}^2$. Therefore, the last strict inequality holds. x_4' and x_5' can be chosen freely, and we have shown that $c_i(x') > 0$ for all $i \in \mathcal{I}$ for

$$x' = \left(\frac{(\underline{\lambda} + \overline{\lambda}}{2}, \sqrt{\frac{(x_1'x_3' - \underline{\lambda}^2}{2}}, \frac{\underline{\lambda} + \overline{\lambda}}{2}, x_4', x_5'\right) \tag{28}$$

Since it satisfies all the constraints, x' is obviously a feasible point, and we have shown that the constraints satisfy Slater's constraint qualification.

KKT

By the argumentation on the course webpage, the KKT conditions are necessary for local optimality. Since the objective function is convex, they are necessary for global optimality. The KKT conditions are sufficient for global optimality when the objective function is a convex function, the inequality constraints are continuously differentiable concave functions, and the equality functions are affine. This holds in our case.

Question 4

With no equality constraints, the KKT conditions are:

$$\nabla_x \mathcal{L}(x^*, \lambda^*) = \nabla \hat{f}(x^*) - \begin{bmatrix} \lambda_1^* - \lambda_2^* + \lambda_5^* x_3 \\ -2\lambda_5^* x_2 \\ \lambda_3^* - \lambda_4^* + \lambda_5^* x_1 \\ 0 \\ 0 \end{bmatrix} = 0 \tag{29}$$

$$c_i(x^*) \geq 0 \quad \forall \ i \tag{30}$$

$$\lambda_i^* \geq 0 \quad \forall \ i \tag{31}$$

$$\lambda_i^* c_i(x^*) = 0 \quad \forall \ i \tag{32}$$

Question 5

We have implemented the log-barrier algorithm and the BFGS line search algorithm to solve this problem. We have implemented the KKT conditions stated in task 4 as stopping criteria. We use a backtracking line search algorithm for determining step length. In this algorithm, we check for sufficient decrease. We also check that the step we are about to take is in the feasible set, so that we never leave the feasible set if we start inside it. This is also taken care of by using the interior point from Question 4. Since the Wolfe conditions are not necessarily fulfilled, we also check if it is ok to update the Hessian matrix. We have to this point not encountered cases where it was not ok to update it.

We now discuss some solutions. First, a case where the optimal solution can be obtained, since the points are classified with an ellipse that satisfies the constraints. For our first two examples, $\underline{\lambda} = 0.1$ and $\overline{\lambda} = 10$. In figure 1 the points are classified by a circle when letting $A_{\text{classification}}$ be the identity matrix and b the zero vector. The axis scaling makes it look slightly elliptic. The achieved solution is $A_{\text{solution}} = \begin{bmatrix} 1.00800 & 7.12805\text{e}{-04} \\ 7.12805\text{e}{-04} & 1.01748 \end{bmatrix}$. Figure 2 shows the solution where the points are classified by an ellipse, $A_{\text{classification}} = \begin{bmatrix} 1 & 0.3 \\ 0.3 & 0.4 \end{bmatrix}$.

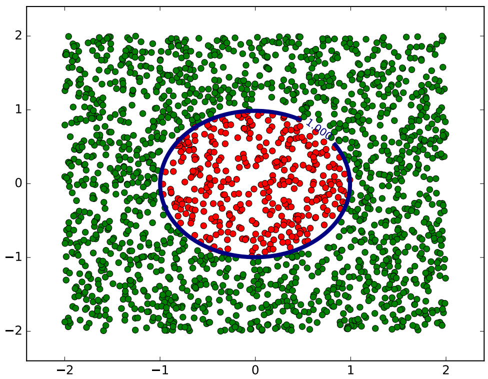

Figure 1: $A_{\text{classification}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$.

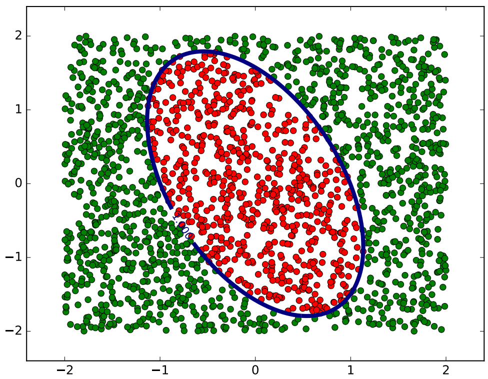

Figure 2: $A_{\text{classification}} = \begin{bmatrix} 1 & 0.3 \\ 0.3 & 0.4 \end{bmatrix}$.

Next, examples where the constraints will limit the size of the matrix entries of the solution. $A_{\text{classification}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. In figure 3, $\underline{\lambda} = 2, \overline{\lambda} = 10$. Here, the solution is $A_{\text{solution}} = \begin{bmatrix} 2.00135 & 0.06451 \\ 0.06451 & 2.00076 \end{bmatrix}$. Note that A_{11} and A_{22} are near but greater than $\underline{\lambda}$, so the solution lies close to constraints c_1 and c_3. The eigenvalues of this matrix are 2.06556894 and 1.9365377. The last one is less than $\underline{\lambda} = 2$, so only the simplified constraints hold, and not those from Question 1. Figure 4 shows an upper size bound example: $\underline{\lambda} = 0.1, \overline{\lambda} = 0.6$, in 14, with solution $A_{\text{solution}} = \begin{bmatrix} 0.59998 & -0.03233 \\ -0.03233 & 0.59998 \end{bmatrix}$. Now A_{11} and A_{22} are near but smaller than $\overline{\lambda}$ so the solution lies close to the constraints c_2 and c_4.

If we classify the points by a hyperbola as in figures 5 and 6, an optimal unconstrained solution would require negative eigenvalues. $A_{\text{classification}} = \begin{bmatrix} 0.0001 & 10 \\ 10 & 0.0001 \end{bmatrix}$, with eigenvalues 10.001 and -9.9999. In figure 5 we let $\underline{\lambda} = 0.01, \overline{\lambda} = 10$. The solution is a very wide ellipse, making the lines almost parallel. $A_{\text{solution}} = \begin{bmatrix} 0.48837 & 0.46210 \\ 0.46210 & 0.45773 \end{bmatrix}$. When adding constraints on size ($\underline{\lambda} = 0.5, \overline{\lambda} = 10$) in figure 6, we get the solution $A_{\text{solution}} = \begin{bmatrix} 0.66799 & 0.43391 \\ 0.43391 & 0.65612 \end{bmatrix}$.

Trouble with terminating BFGS and fulfilling the KKT conditions

In some hard cases, the code had trouble terminating BFGS, and was sometimes unable to satisfy the KKT conditions. If the optimal solution lies close to one or several barriers, ∇P will increase greatly in the direction of the barrier if one passes the bottom of the P function. If the objective function increases a lot in a direction away from the barrier, then the P function may look like a steep "valley" close to the barrier. This is particularly true if we are close to several barriers. When the bottom point is very narrow, it may be very hard for the BFGS algorithm to arrive at a place that is "flat enough" ($\nabla P \leq \tau$, that is). Even the smallest step length passes the very narrow minimum. In our backtracking linesearch

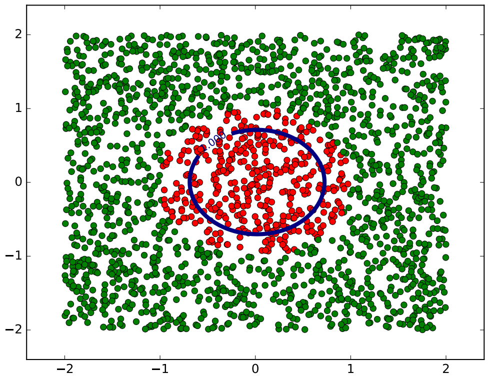

Figure 3: $\underline{\lambda} = 2, \overline{\lambda} = 10$.

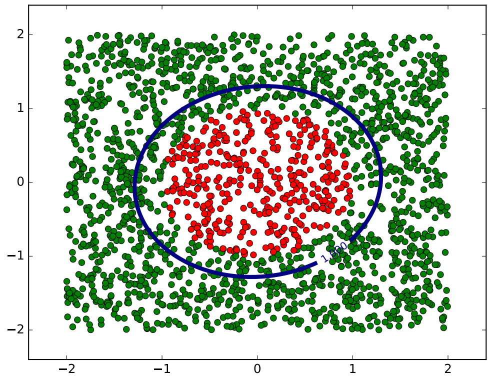

Figure 4: $\underline{\lambda} = 0.1, \overline{\lambda} = 0.6$.

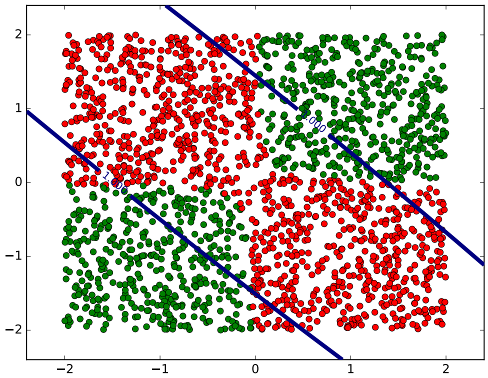

Figure 5: $\underline{\lambda} = 0.01, \overline{\lambda} = 10$.

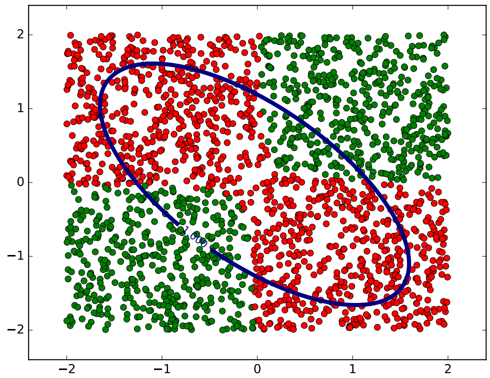

Figure 6: $\underline{\lambda} = 0.5, \overline{\lambda} = 10$.

algorithm we check for sufficient decrease, and if this cannot be achieved the step length is practically reduced to zero. We have therefore implemented an alternative stopping criteria in BFGS, when the step size $\alpha < 1\text{e} - 7$.

When the algorithm is stuck in one place, decreasing μ does not help satisfy the KKT conditions since the size of the column vector from the first KKT condition will decrease, and it is $\nabla \hat{f}$ that is too big. We therefore also have a stopping criteria on $\mu < 1\text{e} - 10$. Based on our plots it seems that these extra conditions result in good solutions.

One case where KKT was not fulfilled was classification by a hyperbola where the vertices of the hyperbola are close to the asymptotes. In figure 7, $\underline{\lambda} = 0.1, \overline{\lambda} = 10$, and again we get the large ellipse. Here, the KKT are still satisfied. In figure 8, we add size constraints: $\underline{\lambda} = 0.5, \overline{\lambda} = 10$. Here, the code does not satisfy the KKT criteria but instead exits when μ gets small enough. The result looks very reasonable though.

The alternative stopping criteria was also needed in thes next examples, where $\underline{\lambda}$ is quite high. For example, with a new "slacker" hyperbola and $\underline{\lambda} = 1, \overline{\lambda} = 10$, the KKT conditions were not satisfied, but the endpoint of the iteration is shown in 9. It looks very reasonable. The same thing also happened for ellipses when $\underline{\lambda}$ was increased. In figure 10, $\underline{\lambda} = 3$. Here, the tilt in the ellipse is unexpected, but not way off.

Lastly, let's look at some misclassification problems. Figure 11 shows a case of 10% misclassification. The KKT conditions are fulfilled and the solution looks reasonable from our experience in the previous project. In figure 12 the misclassification rate is 2%. In both of these plots the circle looks unnaturally big but is correct since the penalty of misclassified points increases with the distance.

What happens if we make $\underline{\lambda}$ and $\overline{\lambda}$ very similar, say $\underline{\lambda} = 0.44, \overline{\lambda} = 0.45$? In this case the KKT

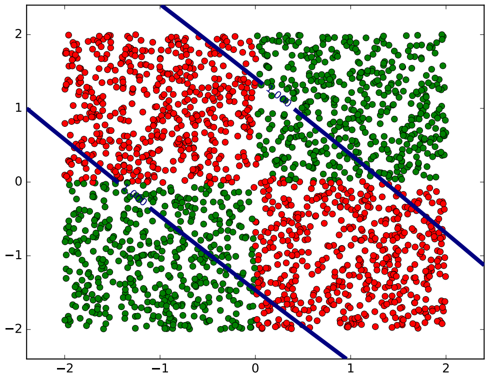

Figure 7: $\underline{\lambda} = 0.1, \overline{\lambda} = 10$. Here, KKT is satisfied.

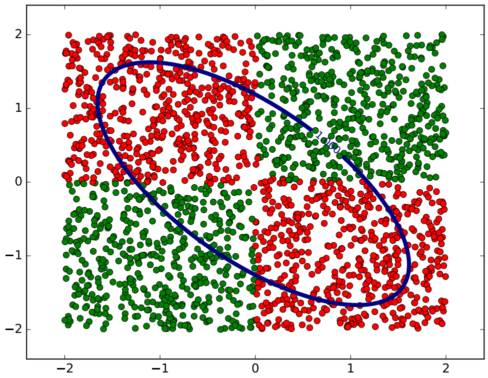

Figure 8: $\underline{\lambda} = 0.5, \overline{\lambda} = 10$. Here, KKT is NOT satisfied.

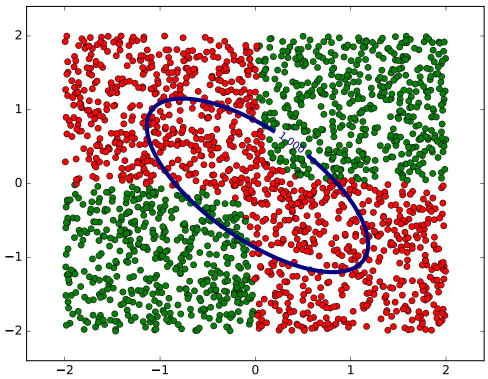

Figure 9: $\underline{\lambda} = 1, \overline{\lambda} = 10$. Here, KKT is not satisfied.

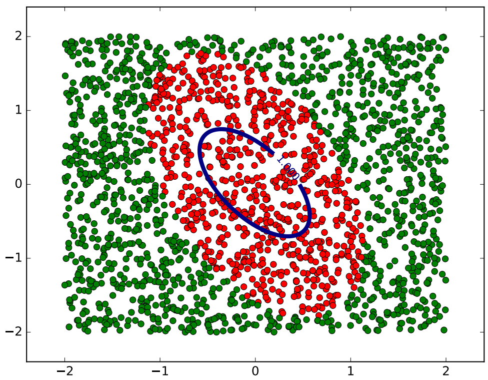

Figure 10: $\underline{\lambda} = 3, \overline{\lambda} = 10$. Here, KKT is not satisfied.

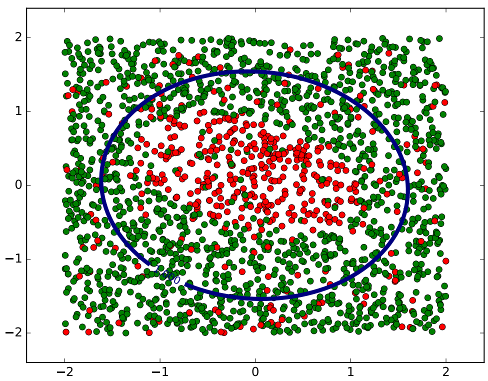

Figure 11: 10% misclassification.

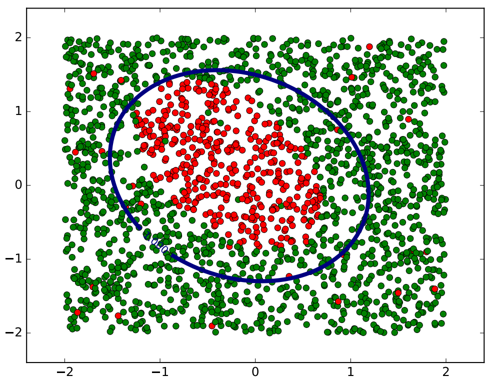

Figure 12: 2% misclassification

conditions were also not satisfied. Here, we see the equal size of the solution for two very different problems: figure 13 and 14. Look at figure 13. The optimal solution should be more tilted and slimmer. This is not allowed though, due to the strict constraints on the matrix entries.

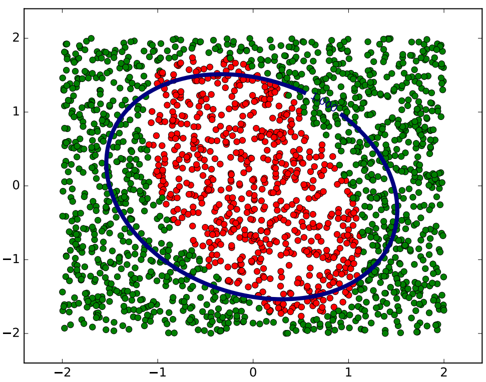

Figure 13: $\underline{\lambda} = 0.44, \overline{\lambda} = 0.45$. KKT not satisfied. Terminating because of small μ.

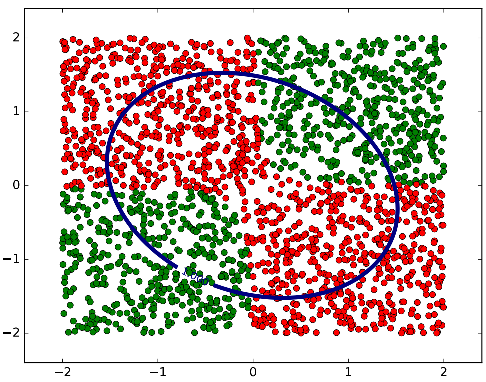

Figure 14: $\underline{\lambda} = 0.44, \overline{\lambda} = 0.45$. KKT not satisfied. Terminating because of small μ.

What happens if we let $\underline{\lambda}$ approach zero? If $\overline{\lambda}$ stays high, it doesn't seem to affect the solution. In figure 15 we have $\underline{\lambda} = 1\mathrm{e}-12, \overline{\lambda} = 2$, and KKT conditions are satisfied. If we let $\overline{\lambda}$ approach zero as well, however, the problem becomes harder. Figure 16 shows a case where $\underline{\lambda} = 1\mathrm{e}-12, \overline{\lambda} = 0.3$, and the KKT conditions were not satisfied.

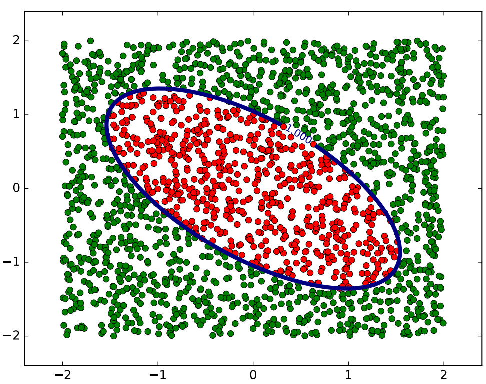

Figure 15: $\underline{\lambda} = 1\mathrm{e}-12, \overline{\lambda} = 2$. KKT is satisfied.

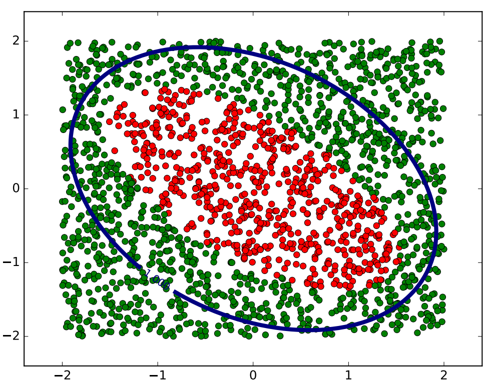

Figure 16: $\underline{\lambda} = 1\mathrm{e}-12, \overline{\lambda} = 2$. KKT not satisfied. Terminating because of small μ.

Conclusion

In general, the algorithm works well, but in cases where the solution lies close to constraints, extra stopping criteria are necessary.