Thanks for helping.

But now I am really more confused about the algorithm that I want to make. Hm.. I have another one question, till now. In a paper the author break the positive defined matrix $G = G^{1/2} G^{1/2}$ and define the matrix $G^{1/2}$ as $G^{1/2} = \Gamma \Lambda^{1/2} \Gamma^T$.

My question is: $\Lambda^{1/2} = \sqrt{\Lambda}$? If that so, and the matrix Λ is a diagonal matrix whose elements are eigenvalues of G, and these eigenvalues are negative, then sqrt(Λ) give complex numbers -unacceptable here.

Now, the author defines G as positive symmetric via type:
$g_{ij} = \frac{1}{2\pi\sigma^2} \exp(-|P_i - P_j|^2 / 2\sigma^2)$ where $|P_i - P_j| = \sqrt{(k-k')^2 + (l-l')^2}$, P → P(k,l).
and say that this is a Positive Definite function (that means it give Positive Definite matrix G (g_{ij}) I guess).

Suppose we have 625 points in a 2D space (P_i, i = 1,...,625, P → P(k,l)).
Then $|P_i-P_j|$ for every i,j between 1 to 625, will lead to a 625x625 diagonal symmetric matrix, say $DM_{625x625}$. The diagonal numbers of $DM_{625x625}$ will be all zero, $|P_i-P_i| = 0$, the others will express the Euclidean Distance between points P_i and P_j, as defined above. $DM_{625x625}$ is generally called as Distance Matrix, having all the relative pairwise distances among all the 625 points in the 2D space.

Having that matrix (DM), I replace the above equation to take the G matrix:

$$g_{ij} = \frac{1}{2\pi\sigma^2} \exp(-|P_i - P_j|^2 / 2\sigma^2) \quad \rightarrow \quad G = \frac{1}{2\pi\sigma^2} \exp(-DM^2_{625x625} / 2\sigma^2)$$

Is what I did correct?

If yes, then G should be a positive definite function, and $\Lambda_{625x625}$ should have the real positive eigenvalues of G (on it's diagonal). But Λ has negative values too! :/ More specific the minimum eigenvalue is -1.7907e-015 for my data. Almost zero, but still negative! :/

Any idea, what I might do wrong?