

Numerical Calculation of the Peak Density Integral in two Squared-Gaussian Fields

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1 Background

In a series of three write-ups FIXME CITE, Professor Guth (and earlier, Saarik Kalia) has written down integral formulations of the expected spatial number density of both minima and stationary points in a sum-of-squares gaussian field ($\Phi = \phi_1 + \phi_2$). The general tactic is similar to the approach in BBKS (FIXME cite bbks). The integrand contains a delta function in the gradient of Φ and a delta function enforcing the constraint that ϕ_1 attain a value some number of standard deviations away from the field mean (zero): $\phi_1 = \nu\sigma_0$, where σ_0 is the standard deviation in ϕ_1 . Additionally, the function contains a factor of the determinant of the hessian matrix of Φ to compensate for the Jacobian factor from the delta-gradient integration. Cancelling out the Jacobian forces the delta function to contribute a value of ± 1 whenever the gradient-delta fires at a stationary point. The sign of the contribution will be addressed shortly. Two central techniques are employed to beat the problem into a useful shape. The first is a rotation in field-space, which will remain an important method as the number of fields is increased. If one envisions ϕ_1 and ϕ_2 as the coefficients of a pair of orthonormal basis vectors in a plane, then the expression $\Phi = \phi_1^2 + \phi_2^2$ is invariant under rotations in this plane. Consequently, the fields can be rotated so that only ϕ_1 is non-zero, and the rotational invariance of our problem implies that the rotated coordinates are just as good as the original ones, so we are able to set ϕ_2 to zero, greatly simplifying our expression (though the gradient of ϕ_2 is not generally zero, and will play a role in the calculation of the hessian matrix of Φ).

The second technique is a transformation into the eigenbasis of the hessian matrix. This allows us to calculate in terms of curvature eigenvalues and rotation matrices (which constitute variable transformations of unit jacobian, and are therefore integral-friendly). Without descending into too much detail (which is nicely worked out in the write-ups), direct control of the eigenvalues allows us to restrict ourselves to minima (all positive eigenvalues), maxima (all negative), or arbitrary saddle-point mixtures. The physically interesting quantity is the number density of field minima, so we will integrate over the positive octant of $[\lambda_1, \lambda_2, \lambda_3]$ space, where the lambdas are these curvature eigenvalues. Our density is independent of the rotation matrices which map this eigen-space onto our physical 3-space, so their euler angles integrate out trivially to a prefactor.

The final step is to calculate the expectation of this density integral over all possible field configurations. We have boiled the density integral down to the value of ϕ_1 ($\nu\sigma_0$), the hessian eigenvalues $\lambda_1 - \lambda_3$, and the gradient components of ϕ_2 : $\eta_1 - \eta_3$. Instead of integrating over 3-space to calculate the total number of minima, we will leave the spatial integrals off and instead integrate over the configuration parameters λ_i and η_j , yielding an expectation of number density. Our field is gaussian, so the joint pdf of these 6 parameters is a multivariate gaussian with covariance matrix calculated in detail in FIXME cite. Putting all of this together yields the following formula from FIXME cite.

$$\begin{aligned} \langle X \rangle_{Q_2} = & \frac{30,375\sigma_0^6}{16\sqrt{30}\pi^{5/2}\kappa^5\sigma_1^{15}e^{-\nu^2/2}\sqrt{\kappa^2-1}} \times \int_{-\infty}^{\infty} d\lambda_1 \int_{-\infty}^{\lambda_1} d\lambda_2 \int_{-\infty}^{\lambda_2} d\lambda_3 (\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_3) \\ & \times \int_{-\infty}^{\infty} d\eta_3 \int_{-\infty}^{\infty} d\eta_2 \int_{-\infty}^{\infty} d\eta_1 \times e^{-Q_2} \end{aligned} \quad (1)$$

Where:

$$Q_2 = \frac{1}{2}\nu^2 + \frac{3}{2\sigma_1^2} \sum_i \eta_i^2 \frac{5\sigma_0^2}{4\kappa^2\sigma_1^4} \left[3 \left(\sum_i \lambda_i^2 - \frac{2}{\nu\sigma_0} \sum_i \lambda_i \eta_i^2 + \frac{1}{\nu^2\sigma_0^2} \left(\sum_i \eta_i^2 \right)^2 \right) - \left(\sum_i \lambda_i - \frac{1}{\nu\sigma_0} \sum_i \eta_i^2 \right)^2 \right] \\ \frac{1}{2\sigma_0^2(\kappa^2 - 1)} \left[\nu\sigma_0 + \frac{\sigma_0^2}{\sigma_1^2} \left(\sum_i \lambda_i - \frac{1}{\nu\sigma_0} \sum_i \eta_i^2 \right) \right]^2 \quad (2)$$

In 1, the integral is taken over \mathbb{R}^3 in η , but is taken over an ordered subspace of \mathbb{R}^3 in λ . This is an enforcement of the restriction:

$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \quad (3)$$

Only after choosing such an ordering of eigenvalues can one guarantee unique “diagonal” decomposition of the hessian into a product of $SO(3)$ matrices and eigenvalues. Without this ordering in place, there is a multiplicity factor of $\frac{1}{3!}$ that appears in front of the integral.

2 Attempts at an Analytic Solution

2.1 Multivariate Gaussian Integrals

Ideally, we would like to find a fully analytic solution to this integral. Its form is reminiscent of a gaussian integral in multiple variables. Such integrals are actually quite simple to evaluate analytically. Consider the following:

$$\int_{\mathbb{R}^N} d^N x \exp\left(-\frac{1}{2}\vec{x}^T \Sigma^{-1} \vec{x}\right) \quad (4)$$

If we want this integral to converge, Σ^{-1} must be positive-definite, which is guaranteed if Σ is indeed a covariance matrix. The inner product of \vec{x} through Σ^{-1} yields a quadratic polynomial homogeneous in x_i , which is exactly what we need for a general multivariate gaussian. Untangling this polynomial appears to be a particularly horrible task, but the trick is to diagonalize. As Σ is a symmetric matrix, so must be its inverse:

$$\begin{aligned} (\Sigma \Sigma^{-1})^T &= \mathbb{I} \\ (\Sigma^{-1})^T \Sigma &= \mathbb{I} \\ \therefore (\Sigma^{-1})^T &= \Sigma^{-1} \end{aligned}$$

the (real) spectral theorem tells us that the diagonal decomposition:

$$\Sigma^{-1} = R^T D R \quad (5)$$

yields R from $SO(N)$, so we may change basis into the eigenbasis of Σ^{-1} with unit jacobian. Furthermore, a covariance matrix and its inverse are both positive-definite, so $D = D^{1/2} D^{1/2}$. We may change variables:

$$\vec{x} \rightarrow \vec{u} = D^{1/2} R \vec{x} \quad (6)$$

And now 4 becomes:

$$\frac{1}{|\Sigma^{-1}|^{1/2}} \int_{\mathbb{R}^N} d^N u \exp\left(-\frac{1}{2}\vec{u}^T \vec{u}\right) \quad (7)$$

Which can be separated and re-written:

$$\frac{1}{|\Sigma^{-1}|^{1/2}} \prod_{i=1}^N \int_{\mathbb{R}} du_i \exp\left(-\frac{1}{2}u_i^2\right) \quad (8)$$

Performing the canonical integration:

$$\frac{1}{|\Sigma^{-1}|^{1/2}} \prod_{i=1}^N \int_{\mathbb{R}} du_i \exp(-\frac{1}{2}u_i^2) = (2\pi)^{N/2} |\Sigma|^{1/2} \quad (9)$$

Polynomial prefactors of the exponent can be obtained by parameter-differentiation, so this technique is quite general.

The remaining complication is an in-homogeneous polynomial in the exponent. To order 2, this means there may be linear terms. There is a nice trick (variable change) to address this case. What follows is an adaptation of FIXME Cite.

Say we find the following integral:

$$\int_{\mathbb{R}^N} d^N x \exp(-\frac{1}{2} \vec{x}^T \Sigma^{-1} \vec{x} + \vec{J}^T \vec{x}) \quad (10)$$

Which has the additional linear terms: $\vec{J}^T \vec{x}$. The trick is the change of variables:

$$\vec{x} = \Sigma \vec{J} + \vec{\tilde{x}}$$

The integral becomes, on change-of-variables:

$$\exp\left(\frac{1}{2} \vec{J}^T \Sigma \vec{J}\right) \int_{\mathbb{R}^N} d^N \tilde{x} \exp\left(-\frac{1}{2} \vec{\tilde{x}}^T \Sigma^{-1} \vec{\tilde{x}} + \vec{J}^T \vec{\tilde{x}}\right) \quad (11)$$

The new integrand has a homogeneous polynomial in its exponent, and will therefore yield to the same separation as 4.

3 Lambdas First

With these techniques in hand, let us examine our density integral, 1 and it's exponent, 1. The first thing to notice is that Q_2 is quadratic in λ , but quartic in η . Since the gaussian tricks above do not apply to a quartic polynomial, there is no obvious way to proceed in 6 dimensions. This roadblock suggests that we try one of the 3 dimensional subspaces (one accorded to the the three λ and the other to the three η), treating variables from the other as constants. Since the λ only appear to order 2, let's start there. Treating the η as constants, Q_2 is an inhomogeneous polynomial of order 2 in η , and so should be amenable to the diagonal separation from above.

Indeed, it is possible to diagonalize the matrix which generates this polynomial, and to change variables to the eigenbasis. Unfortunately, we are only interested in field minima, and so our λ integrals are not taken over all space. To simplify the limits of integration, we can forget the ordering of λ_i and simply integrate each λ over $[0, \infty)$. If we were integrating in only one λ dimension, we could cast the integral as an evaluation of the gamma function:

$$\Gamma(t) = \int_0^\infty x^{t-1} e^{-x} dx \quad (12)$$

Unfortunately, because of the linear terms (a constant vector shift as variable change: 6) and the diagonalization rotation, the limits of integration are no longer simple, even neglecting the λ ordering. Call the new variables u_1 , u_2 , and u_3 , in which the polynomial exponent becomes $-\frac{1}{2}(u_1^2 + u_2^2 + u_3^2)$. The limits of integration, even without linear terms, define a parallelepiped in 3-space which is bounded on three faces, and extends infinitely to cover what is a distortion (non- $SO(3)$) linear mapping of the positive octant. The issue is, while R may be an orthogonal operator, $D^{1/2}R$ is not, so the limits of integration of u_3 will be a linear function of u_1 and u_2 . u_2 will be a linear function of u_1 , and u_1 will be free. Now that the limits of the innermost integral are no longer 0 and ∞ , there is no gamma-function trick available. The innermost integral yields an error function in the next two variables. One integral can be done, as the integrals of e^{-x^2} can be expressed in terms of error functions:

$$\int du_1 \operatorname{erf}(u_1) = \frac{e^{-u_1^2}}{\sqrt{\pi}} + u_1 \operatorname{erf}(u_1) \quad (13)$$

And the diagonalized integrand can be expressed as the product: $\exp(-\frac{1}{2}u_1^2) \exp(-\frac{1}{2}u_2^2) \exp(-\frac{1}{2}u_3^2)$, so the integral can be partially factored:

$$A \int_{D1} du_1 \exp(-\frac{1}{2}u_1^2) \int_{D2(u_1)} du_2 \exp(-\frac{1}{2}u_2^2) \int_{D3(u_1, u_2)} du_3 \exp(-\frac{1}{2}u_3^2) \quad (14)$$

Where A is a prefactor depending only on η and ν , and $D1, D2, D3$ are domains of integration corresponding to the parallelepiped volume, with $D2(u_1)$ a function of u_1 , and $D3(u_1, u_2)$ is a function of u_1 and u_2 . These domains should be half-infinite, with either upper or lower bounds, depending on the nature of the variable transformation. We will call the finite bounds $l_3(u_1, u_2)$, $l_2(u_1)$, and l_1 respectively, where $l_i()$ is an affine transformation of its input vector (linear with constant offset) resulting from the origin-shifts and non-orthogonality of the planes partially bounding the integration parallelepiped.

So we can proceed by evaluating the u_3 integral in ???. Unfortunately, evaluating the corresponding antiderivative over the half-infinite interval $D3$ yields a term of the form: $\frac{e^{-l(u_1, u_2)^2}}{\sqrt{\pi}} + l(u_1, u_2) \text{erf}(l(u_1, u_2))$. If we then attempt the u_2 integral, we need to evaluate the antiderivative:

$$\int du_2 \exp(-\frac{1}{2}u_2^2) \left(\text{erf}(-l(u_1, u_2)) \sqrt{\pi} + l(u_1, u_2) \text{erf}(l(u_1, u_2)) \right)$$

And here we spot the cloven hoof. Even the relatively simple function:

$$\exp(-x^2) \text{erf}(x + c) \quad (15)$$

does not appear to have an anti-derivative. Consulting an impressive compendium of error-function integrals and antiderivatives [FIXME CITE OWEN](#), provides expressions for similar integrals, but they must be taken over particular domains, and I was unable to translate our complicated case (with nested scaling and shift in the erf arguments) into any of these special representations, although that does not mean it is not possible. It is not obvious to me how to proceed, so let us turn to the η integrals and see if any progress can be made there.

3.1 Eta Integrals

$$Q_2 = \frac{1}{2}\nu^2 + \frac{3}{2\sigma_1^2} \sum_i \eta_i^2 \frac{5\sigma_0^2}{4\kappa^2\sigma_1^4} \left[3 \left(\sum_i \lambda_i^2 - \frac{2}{\nu\sigma_0} \sum_i \lambda_i \eta_i^2 + \frac{1}{\nu^2\sigma_0^2} \left(\sum_i \eta_i^2 \right)^2 \right) - \left(\sum_i \lambda_i - \frac{1}{\nu\sigma_0} \sum_i \eta_i^2 \right)^2 \right] \\ \frac{1}{2\sigma_0^2(\kappa^2 - 1)} \left[\nu\sigma_0 + \frac{\sigma_0^2}{\sigma_1^2} \left(\sum_i \lambda_i - \frac{1}{\nu\sigma_0} \sum_i \eta_i^2 \right) \right]^2$$

The η integrals are, by turns, more and less friendly than the λ integrals. On one hand, the Q_2 polynomial (1, reprinted above for convenience) is quartic in η_i , which complicates things. On the other, the domain of integration is all of \mathbb{R}^3 , which is encouraging, because it suggests that we might be able to avoid the nested-erf roadblock from the lambda integrals. Two angles of attack will be discussed here.

3.1.1 Change of Variables

Although Q_2 is quartic in η_i , there are no linear or cubic terms. Furthermore, η_i only enters as η_i^2 . Consequently, we may rewrite the η -dependent form of Q_2 in inner-product notation in terms not of $\vec{\eta}$, but rather $\vec{\eta}^2 = (\eta_1^2, \eta_2^2, \eta_3^2)$.

$$Q_2 = -\frac{1}{2} \left(\vec{\eta}^2{}^T \mathbf{M} \vec{\eta}^2 + \mathbf{J}^T \vec{\eta}^2 + c \right) \quad (16)$$

Exploiting the convenient representation of the η_i^2 in a vector format, we perform a change of variables.

$$v_i = \eta_i^2$$

This is a transformation, component-wise, of the $\vec{\eta}^2$ vector into a vector \vec{v} .

This transformation yields the jacobian matrix:

$$\frac{\partial v_i}{\partial \eta_j} = 2 * (v_i)^{1/2} \delta_j^i \quad (17)$$

Incorporating the corresponding jacobian factor, the eta integrals become, on change-of-variables:

$$\exp\left(\frac{1}{2}\vec{J}^T \Sigma J\right) \int_0^\infty dv_1 \int_0^\infty dv_2 \int_0^\infty dv_3 (64v_1 v_2 v_3)^{-1/2} \exp\left(-\frac{1}{2}\vec{v}^T \Sigma^{-1} \vec{v} + \vec{J}^T \vec{v}\right) \quad (18)$$

To remove the term linear in v_i , we use the trick we applied to 10:

$$\vec{v} = M^{-1} \vec{J} + \vec{\tilde{v}}$$

Which substitution yields:

$$\exp\left(\frac{1}{2}\vec{J}^T M^{-1} J\right) \int_{w_1}^\infty d\tilde{v}_1 \int_{w_2}^\infty d\tilde{v}_2 \int_{w_3}^\infty d\tilde{v}_3 \exp\left(-\frac{1}{2}\vec{\tilde{v}}^T M \vec{\tilde{v}} + \vec{J}^T \vec{\tilde{v}}\right) \quad (19)$$

Where $w_i = (M^{-1})_i^j J_j$

In preparing our integral for diagonalization, we have fallen into the same nested-erf trap as in Section