

Supplementary Information

Magneto-capillary particle dynamics at curved interfaces: inference and criticism of dynamical models

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1 Models of MJP Dynamics

1.1 Base Model

Following Fei et al.,¹ we seek to describe the motion of a magnetic sphere (radius a) moving at the interface of a spherical drop (radius R) due to a time-varying magnetic field $\mathbf{B}(t)$. The dynamics of the rigid particle is governed by Newton's laws of linear and angular motion

$$M \frac{d\mathbf{U}}{dt} = \mathbf{F}_m + \mathbf{F}_h + \mathbf{F}_c \quad (\text{S1})$$

$$I \frac{d\boldsymbol{\Omega}}{dt} = \mathbf{T}_m + \mathbf{T}_h + \mathbf{T}_c \quad (\text{S2})$$

where M and I are the mass and moment of inertia of the (isotropic) particle, \mathbf{U} and $\boldsymbol{\Omega}$ are its linear and angular velocities, and \mathbf{F} and \mathbf{T} describe the various forces and torques acting on the particle.

The magnetic force and torque on the particle are related to its magnetic moment \mathbf{m} as

$$\mathbf{F}_m = \mathbf{m} \cdot \nabla \mathbf{B} = 0 \quad \text{and} \quad \mathbf{T}_m = \mathbf{m} \times \mathbf{B} \quad (\text{S3})$$

Here, we consider a spatially uniform field, in which the field gradient and therefore the magnetic force are identically zero. Moreover, we model the magnetic moment \mathbf{m} as a constant vector directed parallel to the Janus equator that rotates in lock-step with the particle.

The capillary force and torque are assumed to constrain the particle position and orientation as described by the kinematic conditions

$$\mathbf{n} \cdot \mathbf{U} = 0 \quad \text{and} \quad \boldsymbol{\Omega} \times \mathbf{n} = \mathbf{U} \cdot \nabla \mathbf{n} \quad (\text{S4})$$

where \mathbf{n} is the unit vector normal to the drop interface. The particle can translate parallel to the interface and rotate normal to the interface; however, other motions are prohibited. This rigid constraint is appropriate when capillary forces greatly exceed magnetic forces—that is, when $\gamma a^2/mB \gg 1$ where γ is the interfacial tension. For a spherical interface of radius R , the kinematic constraints of equation (S4) can be simplified as

$$\mathbf{U} = R(\boldsymbol{\Omega} \times \mathbf{n}) \quad (\text{S5})$$

At low particle Reynolds numbers ($\text{Re} = \rho U a / \eta \ll 1$), the hydrodynamic force and torque on the particle depend linearly on its linear and angular velocity as

$$\begin{bmatrix} \mathbf{F}_h \\ \mathbf{T}_h \end{bmatrix} = - \begin{bmatrix} \mathbf{R}_{FU} & \mathbf{R}_{F\Omega} \\ \mathbf{R}_{TU} & \mathbf{R}_{T\Omega} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{U} \\ \boldsymbol{\Omega} \end{bmatrix} \quad (\text{S6})$$

where \mathbf{R}_{FU} , $\mathbf{R}_{F\Omega}$, $\mathbf{R}_{T\Omega}$, and \mathbf{R}_{TU} are the components of the hydrodynamic resistance tensor. For small spheres ($a \ll R$) adsorbed symmetrically at the interface between two immiscible liquids of equal viscosity η , the resistance tensors can be approximated as by those of a sphere in a single unbounded fluid

$$\mathbf{R}_{FU} = 6\pi\eta a \boldsymbol{\delta}, \quad \mathbf{R}_{F\Omega} = \mathbf{R}_{TU} = 0, \quad \mathbf{R}_{T\Omega} = 8\pi\eta a^3 \boldsymbol{\delta}, \quad (\text{S7})$$

This approximation is valid only for particles that satisfy the kinematic conditions of equation (S4).

On the time scale of the driving field (i.e., the frequency ω), effects due to particle inertia are negligible when $M\omega/6\pi\eta a \ll 1$ (or, equivalently, when $I\omega/8\pi\eta a^3 \ll 1$). As this condition is well satisfied in the experiments, we neglect the inertial terms on the left hand side of equations (S1) and (S2). The resulting balance of forces implies that the capillary force is proportional to the particle velocity

$$\mathbf{F}_c = 6\pi\eta a \mathbf{U} \quad (\text{S8})$$

where $\mathbf{F}_c \cdot \mathbf{n} = 0$ in accordance with the kinematic constraint (S4). Similarly, the balance of torques implies that

$$\mathbf{T}_c = 8\pi\eta a^3 \boldsymbol{\Omega} - \mathbf{m} \times \mathbf{B} \quad (\text{S9})$$

Magnetic torques directed parallel to the surface normal \mathbf{n} is resisted by viscous friction; those perpendicular to the surface normal are instead resisted by capillary torques that act to prevent deformation of the liquid interface.

To close the system of equations and solve for the particle velocity, we consider that the energy supplied by the magnetic torque is dissipated by particle motion through the viscous fluid

$$\mathbf{T}_m \cdot \boldsymbol{\Omega} + \mathbf{T}_h \cdot \boldsymbol{\Omega} + \mathbf{F}_h \cdot \mathbf{U} = 0 \quad (\text{S10})$$

By contrast, the capillary constraints perform no work on the system. Substituting the kinematic constraint and making use of common vector identities, we obtain

$$\begin{aligned} 0 &= \mathbf{T}_m \cdot \boldsymbol{\Omega} - 8\pi\eta a^3 \boldsymbol{\Omega} \cdot \boldsymbol{\Omega} - 6\pi\eta a R^2 (\boldsymbol{\Omega} \times \mathbf{n}) \cdot (\boldsymbol{\Omega} \times \mathbf{n}) \\ 0 &= (\mathbf{T}_m - 8\pi\eta a^3 \boldsymbol{\Omega} - 6\pi\eta a R^2 (\boldsymbol{\delta} - \mathbf{nn}) \cdot \boldsymbol{\Omega}) \cdot \boldsymbol{\Omega} \\ 0 &= \mathbf{T}_m - 8\pi\eta a^3 \boldsymbol{\Omega} - 6\pi\eta a R^2 (\boldsymbol{\delta} - \mathbf{nn}) \cdot \boldsymbol{\Omega} \end{aligned} \quad (\text{S11})$$

To summarize, the angular velocity of the particle is related to the magnetic torque as

$$\boldsymbol{\Omega} = \left(\frac{\boldsymbol{\delta} - \mathbf{nn}}{8\pi\eta a^3 + 6\pi\eta a R^2} + \frac{\mathbf{nn}}{8\pi\eta a^3} \right) \cdot (\mathbf{m} \times \mathbf{B}) \quad (\text{S12})$$

where the magnetic moment is directed always perpendicular to the interface, $\mathbf{m} \cdot \mathbf{n} = 0$.

Numerical Integration

To integrate the particle dynamics, we introduce two coordinate systems: the world frame and the particle frame.² Vectors expressed in the particle frame (denoted by a prime, \mathbf{B}') are related to the same vector expressed in the world frame as $\mathbf{B}' = R_q(\mathbf{q})\mathbf{B}$ where R_q is the rotation matrix parameterized by the unit quaternion \mathbf{q}

$$R_q(\mathbf{q}) = \begin{bmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2q_0q_2 + 2q_1q_3 & 2q_1q_3 - 2q_0q_2 \\ 2q_1q_2 - 2q_0q_3 & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2q_2q_3 + 2q_0q_1 \\ 2q_1q_3 + 2q_0q_2 & 2q_2q_3 - 2q_0q_1 & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{bmatrix} \quad (\text{S13})$$

In the particle frame, the magnetic moment is constant and directed in the x' direction such that $\mathbf{m}' = [m, 0, 0]^T$; the Janus director is directed in the z' direction. In the world frame, the precessing magnetic field with frequency ω and angle φ is specified as

$$\mathbf{B}(t) = \begin{bmatrix} B \sin \varphi \cos \omega t \\ B \sin \varphi \sin \omega t \\ B \cos \varphi \end{bmatrix} \quad (\text{S14})$$

The quaternion $\mathbf{q}(t)$ characterizing the particle orientation evolves in time as

$$\begin{aligned} \frac{d\mathbf{q}}{dt} &= \frac{1}{2} W'(\mathbf{q})^T \boldsymbol{\Omega}' \\ \frac{d\mathbf{q}}{dt} &= \frac{W'(\mathbf{q})^T}{6\pi\eta a R^2} \begin{bmatrix} (1 + \frac{4a^2}{3R^2})^{-1} & \cdot & \cdot \\ \cdot & (1 + \frac{4a^2}{3R^2})^{-1} & \cdot \\ \cdot & \cdot & (\frac{4a^2}{3R^2})^{-1} \end{bmatrix} (\mathbf{m}' \times \mathbf{B}'(t)) \end{aligned} \quad (\text{S15})$$

where the matrix $W'(\mathbf{q})$ relating the angular velocity to the quaternion rates is given by

$$W'(\mathbf{q}) = \begin{bmatrix} -q_1 & q_0 & q_3 & -q_2 \\ -q_2 & -q_3 & q_0 & q_1 \\ -q_3 & q_2 & -q_1 & q_0 \end{bmatrix} \quad (\text{S16})$$

At time $t = 0$, the particle is positioned at the lower pole of the drop, $\mathbf{x}(0) = [0, 0, -R]$. Its magnetic moment is assumed to point in the x -direction, which corresponds to the preferred alignment in the field at $t = 0$. The initial quaternion is therefore

$$\mathbf{q}(0) = [0, 1, 0, 0]^T \quad (\text{S17})$$

From this initial orientation, equation (S15) for the quaternion rates is integrated numerically in Julia using the KenCarp4 method for stiff ODEs with moderate precision. From the solution, the particle trajectory in the world frame $\mathbf{x} = [x, y, z]$ is given by

$$\mathbf{x}(t) = R_q(\mathbf{q}(t)) [0, 0, R]^T \quad (\text{S18})$$

1.2 Gravity Model

The gravity model augments equation (S1) with an additional force due to gravity

$$\mathbf{F}_g = M\mathbf{g} \quad (\text{S19})$$

where \mathbf{g} is the acceleration due to gravity, and M is the buoyant mass of the particle in the fluid. This additional force is included in the energy balance (S10) to give

$$\mathbf{T}_m \cdot \boldsymbol{\Omega} + \mathbf{F}_g \cdot \mathbf{U} + \mathbf{T}_h \cdot \boldsymbol{\Omega} + \mathbf{F}_h \cdot \mathbf{U} = 0 \quad (\text{S20})$$

Making use of the kinematic constraint, this equation implies that

$$\begin{aligned} 0 &= \mathbf{T}_m \cdot \boldsymbol{\Omega} + R\mathbf{F}_g \cdot (\boldsymbol{\Omega} \times \mathbf{n}) - 8\pi\eta a^3 \boldsymbol{\Omega} \cdot \boldsymbol{\Omega} - 6\pi\eta a R^2 (\boldsymbol{\Omega} \times \mathbf{n}) \cdot (\boldsymbol{\Omega} \times \mathbf{n}) \\ 0 &= (\mathbf{T}_m + R(\mathbf{n} \times \mathbf{F}_g) - 8\pi\eta a^3 \boldsymbol{\Omega} - 6\pi\eta a R^2 (\boldsymbol{\delta} - \mathbf{nn}) \cdot \boldsymbol{\Omega}) \cdot \boldsymbol{\Omega} \\ 0 &= \mathbf{T}_m + R(\mathbf{n} \times \mathbf{F}_g) - 8\pi\eta a^3 \boldsymbol{\Omega} - 6\pi\eta a R^2 (\boldsymbol{\delta} - \mathbf{nn}) \cdot \boldsymbol{\Omega} \end{aligned} \quad (\text{S21})$$

The angular velocity of the particle is related to the magnetic torque and the gravitational force as

$$\boldsymbol{\Omega} = \left(\frac{\boldsymbol{\delta} - \mathbf{nn}}{8\pi\eta a^3 + 6\pi\eta a R^2} + \frac{\mathbf{nn}}{8\pi\eta a^3} \right) \cdot ((\mathbf{m} \times \mathbf{B}) + R(\mathbf{n} \times \mathbf{F}_g)) \quad (\text{S22})$$

Numerical Integration

The particle position and orientation is parameterized by the unit quaternion $\mathbf{q}(t)$, which evolves in time as

$$\frac{d\mathbf{q}}{dt} = \frac{W'(\mathbf{q})^T}{6\pi\eta a R^2} \begin{bmatrix} (1 + \frac{4a^2}{3R^2})^{-1} & \cdot & \cdot \\ \cdot & (1 + \frac{4a^2}{3R^2})^{-1} & \cdot \\ \cdot & \cdot & (\frac{4a^2}{3R^2})^{-1} \end{bmatrix} ((\mathbf{m}' \times \mathbf{B}'(t)) + RM_b(\mathbf{n}' \times \mathbf{g}')) \quad (\text{S23})$$

Here, the unit normal vector in the particle frame is $\mathbf{n}' = [0, 0, 1]^T$. The acceleration due to gravity in the world frame is $\mathbf{g} = [0, 0, -g]^T$, which is rotated into the particle frame as $\mathbf{g}' = R_q(\mathbf{q})\mathbf{g}$. Compared to the base model, the gravity model introduces one additional parameter—namely, the gravitational torque RMg . Equation (S23) is integrated numerically using the same method described for the base model.

1.3 Angle Model

The angle model considers the possibility that the particle's magnetic moment may have components both parallel and normal to the liquid interface. In the particle frame, the magnetic moment is given by

$$\mathbf{m}' = [m \cos \mu, 0, m \sin \mu]^T \quad (\text{S24})$$

where the angle μ describes the particle tilt with respect to the interface. Substituting this expression for the magnetic moment to equation (S15), the particle dynamics is integrated numerically as described for the base model.

1.4 Paramagnetic Model

The paramagnetic model considers that the particle's magnetic moment has additional contributions proportional to the applied field

$$\mathbf{m} = \mathbf{m}_p + \boldsymbol{\alpha} \cdot \mathbf{B} \quad (\text{S25})$$

where \mathbf{m}_p is the permanent magnetic moment, and $\boldsymbol{\alpha}$ is the magnetic polarizability tensor. For a Janus sphere with director \mathbf{n} , the axial symmetry of the particle suggests that the polarizability tensor has the form

$$\boldsymbol{\alpha} = \alpha_{\perp}(\boldsymbol{\delta} - \mathbf{nn}) + \alpha_{\parallel}\mathbf{nn} \quad (\text{S26})$$

Importantly, paramagnetic contributions to the magnetic torque depend only on the difference between the two polarizabilities, $\Delta\alpha = \alpha_{\perp} - \alpha_{\parallel}$. For the purpose of integrating the

particle dynamics, we therefore write the magnetic moment in the particle frame as

$$\mathbf{m}' = \begin{bmatrix} m_p \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} \Delta\alpha & 0 & 0 \\ 0 & \Delta\alpha & 0 \\ 0 & 0 & 0 \end{bmatrix} \mathbf{B}' \quad (\text{S27})$$

Compared to the base model, the paramagnetic model introduces one additional parameter—namely, the polarizability difference $\Delta\alpha$. Substituting this expression for the magnetic moment to equation (S15), the particle dynamics is integrated numerically as described for the base model.

1.5 Correlated Noise

Following Sivia³, we adopt the following likelihood function for the N -dimensional data vector D

$$p(D | \theta, M) = \frac{1}{\sqrt{(2\pi)^N \det(C)}} \exp\left(-\frac{1}{2}(F(\theta) - D)^\top C^{-1}(F(\theta) - D)\right) \quad (\text{S28})$$

where C is the $N \times N$ covariance matrix, and $F(\theta)$ is the N -dimensional vector of model predictions given parameters θ . To describe correlated noise, the covariance matrix C with elements C_{jk} is modeled as

$$C_{jk} = \sigma^2 \exp(-|t_j - t_k|/\tau) = \sigma^2 \epsilon^{|j-k|} \quad (\text{S29})$$

where σ is the noise magnitude, τ is the correlation time, t_j denotes the time of data point j , and $\epsilon \equiv \exp(-\Delta t/\tau)$ for a constant time step $\Delta t = t_{j+1} - t_j$. For a constant time step Δt , the inverse covariance matrix is tridiagonal, and the log-likelihood can be evaluated more quickly as

$$\ln p(D | \theta, M) = \text{constant} - \frac{1}{2} \left[(N-1) \ln(1 - \epsilon^2) + \frac{Q}{1 - \epsilon^2} \right] \quad (\text{S30})$$

where

$$\begin{aligned} Q &= \chi^2 + \epsilon [\epsilon(\chi^2 - \phi) - 2\psi] \\ \chi^2 &= \sum_{k=1}^N R_k^2, \quad \phi = R_1^2 + R_N^2, \quad \psi = \sum_{k=1}^{N-1} R_k R_{k+1} \end{aligned} \quad (\text{S31})$$

Here, $R_k = F_k - D_k$ denotes the residual between the model prediction F_k and the observed datum D_k . Note that the unspecified constant in equation (S30) can be neglected for the purpose of parameter estimation, but must be evaluated explicitly during model selection.

2 Prior distributions

	Parameter	Mean	Std. Dev.
shared	log-magnetic moment, $\log_{10}(m/m_{\text{ref}})$	0.5	1.0
	Drop radius, R	68 px	0.25 px
	Tilt angle, μ	0 rad	0.1 rad
	Polarizability diff., $\Delta\alpha / \Delta\alpha_{\text{ref}}$	2	1
	Log-bouyant mass, $\log_{10}(M/M_{\text{ref}})$	-2	1
per exp.	Initial particle location (x, y)	Trackpy	5 px
	Initial particle orientation	0 rad	3 rad
	Field phase	0 rad	1 rad

Table SI: Summary of priors distributions used. All priors are normally distributed with quoted means and standard deviations. Note that 1 pixel (px) = 0.58 μm . Reference quantities used to scale model parameters are $m_{\text{ref}} = 10^{-14}$ A m², $\Delta\alpha_{\text{ref}} = 4 \times 10^{-12}$ A² m³/N, $M_{\text{ref}} = 3 \times 10^{-14}$ g.

3 Bayesian model selection

We approximate the posterior distributions for each batch by normal distributions such that

$$p(\theta \mid \mathcal{D}_b, M) \propto p(\theta \mid M)p(\mathcal{D}_b \mid \theta, M) \approx C_b \mathcal{N}(\theta \mid \mu_b, \Sigma_b) \quad (\text{S32})$$

where μ_b and Σ_b denote the mean and covariance of the batch posterior obtained by the Laplace approximation for $b = 1, \dots, B$. The constant C_b is identified as the model likelihood $p(\mathcal{D}_b \mid M)$ for the batch-level data \mathcal{D}_b . Assuming a normal prior with mean μ and covariance Σ , the joint posterior conditioned on all batches is also normal

$$p(\theta \mid \mathcal{D}) = \frac{p(\theta \mid M)}{p(\mathcal{D} \mid M)} \prod_{b=1}^B \frac{C_b \mathcal{N}(\theta \mid \mu_b, \Sigma_b)}{p(\theta \mid M)} = \mathcal{N}(\theta \mid \mu_p, \Sigma_p) \quad (\text{S33})$$

with covariance Σ_p and mean μ_p given by

$$\begin{aligned} \Sigma_p &= \left(-(B-1)\Sigma^{-1} + \sum_{b=1}^B \Sigma_b^{-1} \right)^{-1} \\ \mu_p &= \Sigma_p \left(-(B-1)\Sigma^{-1}\mu + \sum_{b=1}^B \Sigma_b^{-1}\mu_b \right) \end{aligned} \quad (\text{S34})$$

The model likelihood can then be expressed as

$$\begin{aligned} p(\mathcal{D} \mid M) &= \frac{|2\pi\Sigma_p|^{1/2}}{|2\pi\Sigma|^{1/2}} \exp \left(-\frac{1}{2}(\mu_p - \mu)^T \Sigma^{-1}(\mu_p - \mu) \right) \\ &\times \prod_{b=1}^B \frac{C_b |2\pi\Sigma|^{1/2}}{|2\pi\Sigma_b|^{1/2}} \exp \left(-\frac{1}{2}(\mu_p - \mu_b)^T \Sigma_b^{-1}(\mu_p - \mu_b) + \frac{1}{2}(\mu_p - \mu)^T \Sigma_b^{-1}(\mu_p - \mu) \right) \end{aligned} \quad (\text{S35})$$

where the first term is the Occam factor, and the second term is the likelihood for \mathcal{D} evaluated for the most probable parameters μ_p .

In practice, we use the parameter estimate of equation (S34) to initialize the gradient-driven optimization of the log-posterior conditioned on all the data—that is, $\ln p(\theta \mid \mathcal{D}, M)$. The resulting optimum is assumed to be the mode of the posterior distribution. The posterior covariance is approximated at this point using the Laplace approximation.

4 Information content of an experiment

Following Lindley,^{3,4} the value of data y in reducing our uncertainty of model parameters θ can be quantified as the Kullback–Leibler (KL) divergence between the posterior and prior distributions

$$u(y) = \int p(\theta | y) \ln \left(\frac{p(\theta | y)}{p(\theta)} \right) d\theta \quad (\text{S36})$$

In the present analysis, both the prior $p(\theta)$ and the posterior $p(\theta | y)$ are approximated by multivariate normal distributions with respective means μ_π and μ_p and covariance matrices Σ_π and Σ_p . The above integral can then be evaluated to obtain

$$u(y) = \frac{1}{2} \left[\ln \frac{|\Sigma_\pi|}{|\Sigma_p|} - d + \text{tr} (\Sigma_\pi^{-1} \Sigma_p) + (\mu_p - \mu_\pi)^T \Sigma_\pi^{-1} (\mu_p - \mu_\pi) \right] \quad (\text{S37})$$

where d is the number of parameters. This expression was used to compute the amount of information gained by analysis of each batch using the favored ag-model.

Batch	Information (bits)
1	4154
2	912
3	676
4	8680
5	1262
combined	11023

Table SII: Information gained from the prior distribution for the favored ag model, for all shared parameters.

5 Implementation details

Source code for the analyses described in this paper can be found at <https://github.com/bishopgroup/MJPinference>. Below, we summarize the packages used and provide code snippets for different elements of the analysis.

5.1 Package versions

Julia v1.8 was used for all statistical analysis. The environment specification is included below.

Package Name	Version
DiffEqBayes	v3.0.0
DiffEqSensitivity	v6.79.0
Distributions	v0.25.70
ForwardDiff	v0.10.32
HypothesisTests	v0.10.11
Interpolations	v0.14.7
LatinHypercubeSampling	v1.8.0
NLOpt	v0.6.5
ODEInterfaceDiffEq	v3.11.0
OrdinaryDiffEq	v6.24.4
StatsBase	v0.33.21

5.2 Code snippets

Correlated Noise (exact)

This function calculates the log-likelihood but is extremely slow due to the matrix inverse operation. It is used for model selection but not for parameter estimation.

```
function get_exact_correlated_LL(r, epsilon, sigma)
    k = length(r)
    C = Matrix([sigma^2 * epsilon^abs(i-j) for i in 1:k, j in 1:k])

    pi_factor = -k/2*log(2*3.14159265359)
    det_factor = -0.5 * (2*k*log(sigma) + (k-1)*log(1-epsilon^2))
    chi_factor = -0.5 * (r' * inv(C) * r)

    return pi_factor + det_factor + chi_factor
end
```

Correlated Noise (proportional)

This function returns the log-likelihood to within an additive constant and is significantly faster than the function above. It is used during optimization to identify the most probable

parameters.

```
function get_proportional_correlated_LL(r, epsilon, sigma)
    #8.34 Sivia
    N = length(r)
    r2 = r .^ 2
    phi = r2[1] + r2[end]
    chi2 = sum(r2)
    psi = sum(r[1:end-1] .* r[2:end])
    Q = chi2 + epsilon * (epsilon * (chi2 - phi) - 2 * psi)
    L = -1 / 2.0 * ((N - 1) * log(1 - epsilon^2) +
        2 * N * log(sigma) + Q / (sigma^2 * (1 - epsilon^2)))
    return L
end
```

z-score

This function evaluates the z-score described by Eq (5) in the main text.

```
function zscore(mu1, Sigma1, mu2, Sigma2, n_par)

    r2min = abs.(mu2[end-n_par+1:end] - mu1[end-n_par+1:end])' *
        inv(Sigma1[end-n_par+1:end, end-n_par+1:end] +
            Sigma2[end-n_par+1:end, end-n_par+1:end]) *
        abs.(mu2[end-n_par+1:end] - mu1[end-n_par+1:end])
    return r2min
end
```

KL Divergence

This function evaluates the KL-divergence between two multivariate normal distributions with means μ_1 and μ_2 and covariance matrices Σ_1 and Σ_2 .

```
function KL(mu1, Sigma1, mu2, Sigma2, n_par)
    #Calculate KL divergence from 1 -> 2, considering n parameters.

    mu1g = mu1[end-n_par+1:end]
    Sigma1g = Sigma1[end-n_par+1:end, end-n_par+1:end]
    mu2g = mu2[end-n_par+1:end]
    Sigma2g = Sigma2[end-n_par+1:end, end-n_par+1:end]

    iSigma2 = inv(Sigma2g)
    kl = 0.5 * (log(abs(det(Sigma2g) / det(Sigma1g))) - n_par +
        tr(iSigma2 * Sigma1g) +
        Transpose(mu2g - mu1g) * iSigma2 * (mu2g - mu1g))

    return kl
end
```

References

1. Fei, W., Tzelios, P. M. & Bishop, K. J. M. Magneto-capillary particle dynamics at curved interfaces: time-varying fields and drop mixing. *Langmuir* **36**, 6977–6983 (2020).
2. Diebel, J. Representing attitude: Euler angles, unit quaternions, and rotation vectors. *Matrix* **58**, 1–35 (2006).
3. Sivia, D. & Skilling, J. *Data Analysis: a Bayesian Tutorial* (Oxford University Press, 2006).
4. Lindley, D. V. On a measure of the information provided by an experiment. *Ann. Math. Stat.* **27**, 986–1005 (1956).