

Inverse Problems: Methods and Applications

N.J. McCORMICK, University of Washington, Mechanical Engineering Department, Seattle, Washington 98195-2600, USA.

Abstract. Inverse problems form the basis of all measurements to the extent that they involve the determination of the cause of a phenomenon based on observations that can be affected by undesired effects such as instrument noise and an imperfect detector response function. There have been solutions of inverse problems in geophysics, medicine, and engineering that have been stimulated by recent developments in the methods used to solve such problems. Some of this work is surveyed with an attempt to classify the methods of solution. The solution methods may be constrained by the type and accuracy of the instrumentation to be used and where it can be located, and whether an active or passive source is available to excite the detector.

1. Introduction

In a typical forward problem of geophysics, engineering, or medicine that can be characterized with a model there are

- one or more governing equations for the field that is to be measured (e.g., a thermodynamic, acoustical, or optical signal),
- properties that constrain the propagation of the field within the medium (e.g., attenuation coefficient or conductivity), and
- boundary conditions and possible internal sources (e.g., a surface albedo or incoming flow of the field quantity).

From this information the field quantity is determined everywhere within the medium at the nodal locations for the solution. As an example one can solve an elementary heat conduction problem in slab geometry governed by the equations

$$\begin{aligned} \rho(x,t)c_p(x,t)\frac{T(x,t)}{\partial t} &= \frac{\partial}{\partial x} \left[k(x,t)\frac{T(x,t)}{\partial x} \right] + S(x,t) , \\ -k(x,t)\frac{T(x,t)}{\partial x} \Big|_{x=0} &= f(t) , \quad t > 0 , \\ T(L,t) &= T_L , \quad t > 0 , \\ T(x,0) &= F(x) , \quad 0 < x < L . \end{aligned} \tag{1.1}$$

Here the temperature $T(x,t)$, as a function of the spatial variable x , $0 \leq x \leq L$, and time t is the desired field quantity in terms of the incoming heat flux $f(t)$ at $x = 0$,

the fixed temperature T_L at the surface $x = L$, the initial temperature distribution $F(x)$, and a spatially distributed source $S(x, t)$. The governing equation for the temperature is a partial differential equation. If the thermal conductivity k , the density ρ , and/or the specific heat c_p depend on $T(x, t)$ then Eq. (1.2) is nonlinear.

For other disciplines the field equation may not be a purely differential equation. A corresponding elementary heat radiation problem in slab geometry for a participating medium is governed by the equations

$$\begin{aligned} & \frac{1}{c} \frac{\partial I(x, \mu, \nu, t)}{\partial t} + \mu \frac{\partial I(x, \mu, \nu, t)}{\partial x} + [\kappa(x, \nu, t) + \sigma(x, \nu, t)] I(x, \mu, \nu, t) \\ &= \int_{\text{all } \nu'} d\nu' \sigma(x, \nu', t) \int_{-1}^1 d\mu' \beta(\mu' \rightarrow \mu, \nu' \rightarrow \nu) I(x, \mu', \nu', t) + \kappa(x, \nu, t) I_b(\nu, T(x, t)), \\ \\ \mu I(0, \mu, \nu, t) &= f(\mu, \nu, t), \quad 0 \leq \mu \leq 1, \quad t > 0, \\ I(L, -\mu, \nu, t) &= 2 \int_{\text{all } \nu'} d\nu' \int_0^1 d\mu' r(\nu' \rightarrow \nu, \mu' \rightarrow \mu) \mu' I(L, \mu', \nu', t), \quad t > 0, \\ I(x, \mu, \nu, 0) &= F(x, \nu), \quad 0 < x < L. \end{aligned} \tag{1.2}$$

Here the radiation intensity $I(x, \mu, \nu, t)$, as a function of the spatial variable x with direction cosine μ , frequency ν , and time t is the desired field quantity. It is a function of the incoming flux $f(\mu, \nu, t)$ at $x = 0$, a reflection condition at the surface $x = L$ governed by the surface reflectivity $r(\nu' \rightarrow \nu, \mu' \rightarrow \mu)$, and the initial intensity distribution $F(x, \nu)$. The term $I_b(\nu, T(x, t))$ denotes the blackbody re-radiation term arising from radiant energy absorbed at a different frequency. The governing equation for the intensity is an integrodifferential equation in terms of the absorption and scattering coefficients $\kappa(x, \nu, t)$ and $\sigma(x, \nu, t)$ and the directionally-dependent scattering phase function $\beta(\mu' \rightarrow \mu, \nu' \rightarrow \nu)$.

With the additional variables μ and ν that are not present in the heat conduction equation, the radiative equation is the more complicated of the two to solve. The radiative transfer equation can be even more difficult if there is a dependence in the boundary conditions on a second variable to describe the direction of radiation, which is the azimuthal angle about the normal to a slab surface. It is also possible to pose a combined conduction-radiation problem in which the source term in the conduction equation arises from absorbed radiation propagating within the medium.

For an inverse problem the field quantity is measured at one or more locations on the boundary or within the medium and one or more characteristics of the problem are estimated, such as the properties of the medium and/or the boundary conditions and/or the internal sources. Thus an inverse problem forms the basis for inferring fundamental data from measurements. Inverse problems are encountered in virtually all areas of science and engineering, although often they are not recognized as such.

Examples of inverse heat conduction problems are the estimation of the incoming heat flux $f(t)$ or the initial temperature profile $F(x)$ or $k(x, t)/[\rho(x, t)c_p(x, t)]$. Examples of inverse radiative heat problems are the estimation of $\kappa(x, \nu, t) + \sigma(x, \nu, t)$ or the incoming flux $f(\mu, \nu, t)$ or the initial intensity $F(x, \mu)$.

A forward problem generally can be written as

$$\begin{aligned} B\psi &= S, & x \in X, t > 0, \\ \psi &= \psi_0, & x \in X, t = 0, \\ \psi &= \psi_{boundary} + \alpha\psi, & x \in X_{boundary}, t > 0. \end{aligned} \quad (1.3)$$

Here we denote the field quantity by $\psi = \psi(x, t; p)$, where x denotes the phase space of variables $x \in X$, such as the (1-, 2-, or 3-variable) spatial position \mathbf{r} , the (0-, 1-, or 2-variable) direction $\mathbf{\Omega}$, and energy E , and t is time. B and α are linear or nonlinear operators. The parameters p that define the forward problem, such as the properties of the medium and all the sources (S , ψ_0 , and $\psi_{boundary}$), are known. The solution of the forward problem for each possible set of parameters p defines an implicit map M of the space of parameters p onto the space of functions ψ ,

$$\psi = Mp. \quad (1.4)$$

In a typical inverse problem, a subset of unknown parameters in p are to be determined from measurements of ψ with a detector whose response function can be modeled with the operator D , thus giving $D\psi = DMp$. In practice this equation has to be understood in the following sense: $D\psi$ can be only approximately measured, as denoted by $\widetilde{D}\psi$. Because M is an implicit map, this leads to an iterative solution for the values of p from

$$\widetilde{D}\psi = DMp. \quad (1.5)$$

However, the solution of this equation may not exist. When $(DM)^{-1}$ does not exist, usually there are an infinite number of possible solutions, in which case the classical approach is to use some form of ‘‘regularization’’ (Tikonov & Arsenin [16]). This is done by selecting one of the solutions by adding an external constraint not contained in the definition of the inverse problem. This amounts to constructing an inverse for DM .

In any case, whether $(DM)^{-1}$ exists or has been obtained by regularization, the solution of the inverse problem,

$$p = (DM)^{-1}\widetilde{D}\psi, \quad (1.6)$$

is usually ill conditioned.

Even with a perfect detector and with measurements of the complete field $\widetilde{\psi}$ so that D is an identity operator, the determination of p can be difficult because M^{-1} may be ill conditioned. Usually the mapping of p in Eq. (1.4) is well conditioned in the sense that small changes in the parameters give small changes in ψ so that

$$\frac{\|\delta\psi\|}{\|\psi\|} < a \frac{\|\delta p\|}{\|p\|}, \quad a > 0 \text{ and } a = \mathcal{O}(1),$$

where, for example, for the L_2 norm

$$\|f\| = \left(\int [f(x)]^2 dx \right)^{1/2},$$

or, if f is of finite dimension,

$$\|f\| = \left[\sum_{i=1} f_i^2 \right]^{1/2} .$$

If mapping (1.4) is well conditioned, then the inverse problem is not and the values of $\|\delta p\|/\|p\|$ become very sensitive to the small errors $\|\delta(D\psi)\|$ arising from $(\widetilde{D\psi}) = D\psi + \delta(D\psi)$.

How does one assess the degree of degeneracy in the solution that results from measured data? This is usually done by performing sensitivity tests to see how strongly each component of p influences the observation. The sensitivity can be visualized by plotting DMp versus the component and examining the slope of the curve: the smaller the slope, the greater the likelihood that the solution of the inverse problem for that component will be highly sensitive to noise in the data. Another way to interpret sensitivity of a solution to an inverse problem is to consider the condition number C that can be expressed in terms of norms as

$$C = \|DM\| \|(DM)^{-1}\| . \quad (1.7)$$

This equation applies in the case when DM is a linear operator; otherwise, the Gateau derivative must be used in $C = \|DM\| \|[(DM)^{-1}]'_\psi\|$. The condition number is usually large when there are many unknowns, which means that errors in the unknowns p may be large; this has been encountered, for example, in the estimation of the coefficients of a Legendre polynomial expansion of the angle-dependent scattering cross section of radiative transfer (Oelund & McCormick [13]).

How does one cope with mild to moderately-severe ill conditioning when considering an inverse problem? One technique is to look for a smaller number of parameters or other parameters that are less sensitive to the errors in the measured data. An example is the use of a ratio of parameters like κ/σ that give a dimensionless variable, rather than the two variables themselves. The idea is to find a combination of parameters that have greater sensitivity coefficients than the parameters themselves.

After I briefly outline in Sec. 2 some of the inverse problems that have been considered in a variety of applications, in Sec. 3 I will illustrate different classification schemes for inverse problems. Then methods of solution will be briefly overviewed in Sec. 4.

2. Overview of Geophysics, Medical, and Engineering Applications

It is hard to adequately describe the plethora of applications where inverse methods have been used. In geophysics the problems range from *in situ*, invasive-detector techniques such as “oil well logging” (which is the depth-dependent sounding for petrochemicals) to seismic tomography. In oceanography typical applications arise

with the *in situ* characterization of sea water (typically for the phytoplankton concentration in open ocean waters or for sediment and pollutants in near-coastal waters) to the characterization of the ocean's temperature for the assessment of global warming. Temperature profiling of the atmosphere (e.g., from weather balloon measurements) is an application in atmospheric sciences. Remote, noninvasive-detectors sometimes are used instead of *in situ* detectors to acquire data from a flyover by an airplane or satellite.

In medicine, many of the modern clinical diagnostic techniques used today, such a computerized tomography or magnetic resonance imaging, involve the solution of inverse problems. Computerized tomography involves the use of ionizing radiation sources such as x-rays or gamma-rays and relies on the assumption of straight-line propagation of the radiation field. But researchers also are investigating optical mammography applications that require analyzing extensive multiple scattering.

Table 1: Inverse problem applications in different engineering disciplines.

Engineering Discipline	Application
Aerospace	Aerodynamic shape optimization
Biomedical	Electrical impedance tomography for imaging Optical coherence tomography
Chemical	Trace chemical concentrations
Civil	Leak location in underground piping systems Flexural rigidity of a beam from deflection measurements Identification of vibrations of piping systems Estimation of hydraulic transmissivity
Computer	Voice recognition Image reconstruction
Electrical	Electromagnetic scattering properties Electric impedance imaging
Mechanical	Thermal conductivity from heat conduction measurements Thermal diffusivity from heat conduction measurements Surface heat flux from heat conduction measurements Thermal contact resistance Cutting temperature estimation from heat conduction measurements Heat flux estimation in thin-layer drying Heat source estimation Mechanical properties of thin films
Metallurgical	Control of the solid-liquid interface during solidification Nonlinear constitutive laws identification from indentation tests

Optical coherence tomography is another example in which light is used for tissue diagnostics. In that case light that is coherently backscattered from structures

within the tissue (to depths of a few millimeters at most) is collected and interfered with light from a reference, which allows measurement of the echo time delay and amplitude of the reflected light for imaging purposes. Magnetic resonance imaging also is an inverse diagnostic method that avoids the use of ionizing radiation.

Optical techniques for dental applications also are being investigated for the detection and imaging of early carious lesions.

The same diversity of applications occurs in a variety of engineering disciplines. Table 1 gives examples of a few topics, many of which have been addressed in recent “Inverse Problems in Engineering” conferences (Zabaras *et al.* [20]; Woodbury [19]).

A number of books are recommended as good references for applications in different disciplines (Beck *et al.* [2]; Bertero & Boccacci [3]; Hensel [4]; Herman [5]; Hestenes [6]; Iyer & Hirahara [7]; Özisik & Orlande [14]; Trujillo & Twomey [17]).

3. Classifications for Inverse Methods

Besides the grouping applications by discipline, as above, there are several possible classification schemes that can be proposed that help place different problems and/or solution methods into some sort of structure. Kubo [9] proposed that inverse problems be classified as (with some re-organization):

1. Material properties determination problems,
2. Sources and forces determination problems,
3. Boundary/initial value determination problems,
4. Shape determination problems,
5. Governing equation(s) determination problems.

Categories 1–4 depend on the medium which may be severely inhomogeneous, moderately inhomogeneous, or spatially uniform. Examples of what is determined in the different problems for the transfer of radiant energy in a participating medium are: the absorption coefficient of the medium (category 1), the blackbody radiation emitted by the medium (category 2), the incident heat flux entering the medium (category 3), and the shape of an object imbedded within the medium (category 4). (The radiative transfer equation is generally accepted as the governing equation for such problems.) Category 5 represents the ultimate difficulty when solving an inverse problem because the governing equation(s) used to define the propagation of the signal containing information is not known, so different models must be tested.

Other categorization schemes exist that are useful when attempting to design an experimental program to solve problems of the type discussed above, as described in Table 2.

Why is it important to consider the type of detectors to be used? Because the number of independent parameters that one can estimate depends on the number and type of detectors, as illustrated in Eq. (1.6). In the most information-specific situation the detector is located in an element of configuration space (in $d\mathbf{r}$ about \mathbf{r} and is directed in an element of solid angle (in $d\Omega$ about Ω); the detector measures energy (in dE about E) in time intervals (in dt about t) or frequencies (in $d\omega$ about ω). A directionally-integrating detector removes some or all of the information contained in the two variables that specify Ω , while a temperature sensor, for example,

Table 2: Considerations when developing a solution to an inverse problem.

- A. Measurement detector(s)
 1. Number (sufficient for any spatial heterogeneities?)
 2. Location
 - 2a. Outside the medium (external)
 - 2b. Inside the medium (*in situ*)
 3. Type
 - 3a. Narrow field of view (collimated)
 - 3b. Broad field of view (angle-integrated)
- B. Source of excitation
 1. Number (sufficient for any spatial heterogeneities?)
 2. Location
 - 2a. Outside the medium (external)
 - 2b. Inside the medium (*in situ*)
 3. Type of activation of signals to be measured
 - 3a. Passive (inherent to problem)
 - 3b. Active (induced in problem)
 4. Time dependence
 - 4a. Steady-state
 - 4b. Pulsed
 - 4c. Oscillatory

removes all the spectral information in the energy variable.

Why is it important to consider the location and type of the excitation of the system? The amount of information that potentially can be extracted from measurement data depends on where the excitation occurs and its characteristics. There are examples where there is an experimental mismatch: for example, if there is a spatially distributed source deep within an object such that the signal undergoes “corruption” from material inhomogeneities (or extensive multiple scattering, in the case of photon propagation), then the signals are masked by the background noise of the system and/or the detectors.

The relative information content that is potentially available is contained in the sensitivity coefficients. The design of any experiment thus should first include an examination of the sensitivity coefficients to determine if the experiment is even worth doing.

4. Some Solution Methods

For complicated problems where there is a significant spatial dependence of the source or the material properties to be determined, one procedure is to use an iterative comparison of the radiation field computed with an assumed source or material property spatial distribution. Then typically the conjugate gradient method or the

Levenberg-Marquardt method is used to solve problems with an *implicit* or iterative approach. Such an inverse problem can be solved by minimizing a least-squares functional or mismatch function (Press [15])

$$\Delta(\mathbf{Y}, \Phi(\mathbf{x})) = \|\mathbf{Y} - \Phi(\mathbf{x})\|^2 = \sum_{k=1}^K [Y_k - \Phi_k(\mathbf{x})]^2, \quad (4.1)$$

where Y_k is the experimental data and, $\Phi_k(\mathbf{x})$ is the output from a computer code that solves the forward problem with input data \mathbf{x} that comprise the set of unknowns to be determined. (I view such a procedure as analogous to hiking in a group of mountains and wishing to get to the lowest nearby valley; the conjugate gradient method attempts to get a hiker headed into the correct nearby valley and in the most vertical, “fall-line” direction.)

Other mismatch functions can be considered besides that in Eq. (4.1), as succinctly described by Mohammad-Djafari [12]. These include the L_p norm,

$$\Delta(\mathbf{Y}, \Phi(\mathbf{x})) = \|\|\mathbf{Y} - \Phi(\mathbf{x})\|_p\|^p = \sum_{k=1}^K [Y_k - \Phi_k(\mathbf{x})]^p, \quad (4.2)$$

a weighted least squares

$$\Delta(\mathbf{Y}, \Phi(\mathbf{x})) = [\mathbf{Y} - \Phi(\mathbf{x})]^t \mathbf{Q} [\mathbf{Y} - \Phi(\mathbf{x})] = \sum_{i=1}^K \sum_{j=1}^K q_{ij} (Y_i - \Phi_i(\mathbf{x})) (Y_j - \Phi_j(\mathbf{x})), \quad (4.3)$$

or a mismatch function based on information theory, such as the Kullback-Leibler “cross-entropy” function (Kullback [10])

$$\Delta(\mathbf{Y}, \Phi(\mathbf{x})) = \sum_{k=1}^K Y_k \ln \left(\frac{Y_k}{\Phi_k(\mathbf{x})} \right). \quad (4.4)$$

Not many inverse transport problems that have been solved with mismatch functions other than the least squares estimate.

An important thing to note is that the cross-entropy function, sometimes also referred to as the “information gain” is more general than least squares and reduces to that case in the limit of small differences between Y_k and $\Phi_k(\mathbf{x})$ (Kullback [10]). For this reason I believe it should be considered for use in a variety of inverse problems.

An alternative iterative method of solving inverse problems is the so-called regularization approach in which the function to be minimized takes the form of

$$\Delta_1(\mathbf{Y}, \Phi(\mathbf{x})) + \lambda \Delta_2(\mathbf{x}, \mathbf{x}_0), \quad (4.5)$$

where \mathbf{x}_0 is a prior solution, and Δ_1 and Δ_2 are two mismatch functions. When the regularization parameter λ is nonzero, the second (“damping”) term tends to force the new estimate of the unknowns, \mathbf{x} , to stray not too far from the previous

estimate. The optimization of the value of λ has received extensive investigation (e.g., the work of Alifanov *et al.*, 1995). If no information is available for the value of x_0 , then selection of $x_0 = 0$ amounts to the usual norm or energy minimization.

The method of generalized cross-validation also can be used to determine the optimal value of λ . This is done by considering a measured signal $d_j = s_j + \epsilon_j$ to consist of the noise-free signal s_j plus noise ϵ_j . The generalized cross-validation approach works by deleting one of the data points and then using the rest of the data to obtain a predicted value against an independent measurement. This is repeated for all the data points to develop a predicted error analysis. The value of λ that minimizes the predicted error is the optimal one.

In contrast to iterative methods for solving inverse problems, for some problems analytic methods can be developed that require no iteration involving solutions of the governing equation for the problem under consideration. For such methods no mismatch function is used since the deterministic methods are derived directly from the governing equation itself, but the problems that one can potentially solve with such an explicit approach typically are much simpler than those with an implicit approach. As an example, such methods may enable one to determine the properties of a spatially uniform material, or perhaps to identify the presence of at most a few spatial nonuniformities, but generally such a method cannot be used to analyze a material with many spatial inhomogeneities. However, an explicit method has the attractive feature that it can give an initial estimate of the unknowns to use in an implicit procedure, thus possibly improving the likelihood that an iterative search will eventually lead to a global minimum rather than a local one. Another attractive feature of an analytic method is that it can be used to derive analytic sensitivity coefficients that more clearly display the functional dependence of the sensitivity coefficients than those computed with traditional iterative approaches.

As an example of a simple analytic algorithm, consider a small, spherically-symmetric source emitting radiation isotropically in all directions into a large homogeneous medium for which the boundaries can be considered to be at a radius of infinity. For a source magnitude Φ_s [W] the equivalent equation to Eq. (1.3) is given in “conservative form” by (Lewis & Miller [8]),

$$\begin{aligned} \frac{\mu}{r^2} \frac{\partial [r^2 I(r, \mu)]}{\partial r} + \frac{\partial}{\partial \mu} \left\{ \frac{[(1 - \mu^2) I(r, \mu)]}{r} \right\} + (\kappa + \sigma) L(r, \mu) \\ = \frac{\sigma}{2} \int_{-1}^1 I(r, \mu') d\mu' + \frac{\Phi_s \delta(r) \delta(\mu - 1)}{8\pi^2 r^2}, \quad r \geq 0. \end{aligned} \quad (4.6)$$

The simplicity of the problem suggests we develop a recursion relation for the spatial moments of the radiance $I(r, \mu)$ by multiplying Eq. (4.6) by $8\pi^2 r^{n+2} P_k(\mu)$ and integrating over $0 \leq r \leq \infty$ and $-1 \leq \mu \leq 1$. The final result for the recursion relation is

$$\begin{aligned} (k+1)(k-n)I_{n-1, k+1} &= k(n+k+1)I_{n-1, k-1} + (2k+1)(\kappa + (1 - \delta_{k,0}\sigma))I_{n, k} \\ &= (2k+1)\Phi_s \delta_{k,0} \delta_{n,0}, \end{aligned} \quad (4.7)$$

where the definition

$$I_{n,k} = 8\pi^2 \int_0^\infty \int_{-1}^1 r^{n+2} P_k(\mu) I(r, \mu) dr d\mu \quad (4.8)$$

has been introduced. (Note the dimensions of the different $L_{n,k}$ moments depend on the index n .)

Use of Eq. (4.7) with $n = k = 0$ and with $n = 2, k = 0$ gives (after use of the $n = k = 1$ result) an equation for the mean square distance of travel, $\langle r^2 \rangle = I_{2,0}/I_{0,0} = 2[\kappa(\kappa + \sigma)]^{-1}$. This simple equation depends only on the properties of the medium and could be used with a small spherically-shaped detector, such as a foil used to measure a neutron or gamma ray capture rate in a nuclear engineering application, so that the detector matches the constraint that $k = 0$. On the other hand, for a detector with a flat collector oriented perpendicular to r , then the directional moments $k = 1$ are applicable. If the source strength Φ_s is known, for example, then (McCormick & Kaskas [11]) $I_{1,1}/\Phi_s = [\kappa(\kappa + \sigma)]^{-1}$. Thus, depending on what type of detector is used and what measurements are made, the same combination of properties of the medium could be determined.

In practice, however, neither of these algorithms is useful with experimental data. Both are very sensitive to the number and locations where measurements of $I(r, \mu)$ are made that are needed to compute $I_{2,0}$ and $I_{0,0}$ or $I_{1,1}$, a limitation that also is true for an iterative method based on the repeated numerical solution of Eq. (4.6). The algorithms also suffer because the scattering in Eq. (4.6) is isotropic, but this limitation can be easily overcome (McCormick & Kaskas [11]). These examples illustrate that a separate analytic inversion algorithm must be developed for each type of detector, whereas with an iterative procedure for solving inverse problems a common computational procedure can be developed independent of the type of detector. Other analytic algorithms for radiative transfer applications, which work much better than the above simple example, are listed at my website, <http://www.me.washington.edu/faculty>.

Once an analytic algorithm has been developed, however, it can be useful in three ways:

1. As a stand alone method for estimating up to a few parameters,
2. To obtain initial starting values in an iterative solution,
3. For adjusting a few parameters at each step in an iterative solution after all parameters have been estimated.

To date analytic algorithms have been applied only as stand alone methods, so further work needs to be done to fully explore their potential.

5. Conclusions

Any measurement problem can, in a sense, be viewed as the solution of an inverse problem in which measured data is to be converted to an estimation of the variable(s) of interest. Diagnostic applications in geophysics, medicine, and engineering are prime examples of inverse problems that have been solved. Both iterative and

analytic algorithms have been described here, but to solve a complicated problem, such as one with a strongly varying spatial dependence of cross sections, then iterative algorithms are necessary.

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