3.3 Gradient Vector and Jacobian Matrix

Overview: Differentiable functions have a local linear approximation. Near a given point, local changes are determined by the linear approximation, which has the structure of a dot product of the change in position with a fixed vector. For vector-valued functions, the corresponding local change is a product of a fixed matrix with the change in position. This vector or matrix plays a central role in multivariable differential calculus. For scalar functions, the vector of derivatives is called the gradient vector, while for vector-valued functions it is called the Jacobian matrix. The corresponding linear transformations are sometimes called the total derivative or the derivative mapping. In this section, the gradient vector field is explored both algebraically and graphically. Jacobian matrices are calculated and the level sets of the corresponding transformations are plotted. The orthogonality of the gradient to the level sets of the function extends from linear functions to differentiable functions.

3.3.1 Linear functions yet again and dot product

In 2D, a homogenous linear scalar function takes the general form:

f(x, y) = A x + B y, where A and B are constants

and, as discussed in Chapter 1, such functions have special properties. In particular, their values are defined everywhere and the level sets are equally spaced parallel lines. The vector $A\mathbf{i} + B\mathbf{j}$ is orthogonal to the level sets. As we move in any particular direction, the function values will typically change by the dot product with the fixed vector (it doesn't change along the level sets!) and the largest change will be in the direction $A\mathbf{i}+B\mathbf{j}$. A direct calculation with x = A and y = B shows that the change in f in that case is exactly $A^2 + B^2$ and clearly positive. Thus the vector $A\mathbf{i}+B\mathbf{j}$ points in the direction of maximal change and the change per step length in that direction is the ratio:

$$\frac{\text{change in } f}{\text{change in distance}} = \frac{A^2 + B^2}{\sqrt{A^2 + B^2}} = \sqrt{A^2 + B^2}$$

which is the magnitude of the vector. In 3D, a similar expression adds a term C z, the level sets become parallel planes, and again the largest positive change in the linear function occurs in the normal direction x = A, y = B, z = C and has magnitude $A^2 + B^2 + C^2$ so the largest rate of change is $\sqrt{A^2 + B^2 + C^2}$. Recall also that in 3-D a linear function is unchanged in two directions within the level set.

Vector notation makes things neater: we can write A x + B y as $\mathbf{v} \cdot \mathbf{r}$ where $\mathbf{v} = A \mathbf{i} + B \mathbf{j}$ and as usual $\mathbf{r} = x \mathbf{i} + y \mathbf{j}$. The 3D version uses similar notation but with each vector having three components. The maximal rate of change is the magnitude

of v and occurs in that direction. Observe that the components of v are the partial derivatives of f when f is linear! Also, for linear functions, changes in outputs are the same no matter where we start and only depend on the changes in inputs, so to find the change in function values we take the dot product $v \cdot u$, which finds the rate of change of f in any fixed direction u.

This leads us to use the linear approximation and the above algebra to determine how differentiable functions behave locally. Recall that the general principle is continuity means locally constant as first approximation, while differentiability refines that to add a linear approximation for the local change.

3.3.2 Gradient vector in 2D and 3D

Using our heuristic of "think locally", we expect that differentiable functions in general will have similar local behavior to their linear approximations. In particular, near a given point \mathbf{r}_0 , the linear approximation to the local change in a scalar function will again have a dot product structure of a vector, now called the **gradient vector**, paired with the change in location. The instantaneous rate of change in any fixed direction will be the dot product of the gradient vector with the direction of the change. The gradient vector is typically denoted ∇f and sometimes as grad(f). The downward pointing triangular vector symbol is called a "*nabla*". The gradient vector points in the direction of maximal change and the maximal rate of change will be the magnitude of the gradient vector. But when we "act globally" we expect that unlike the linear case, the gradient vector will vary as we vary the location \mathbf{r}_0 .

In terms of its components, the gradient vector at (x_0, y_0) is given by the definition:

$$abla f(x_0, y_0) = rac{\partial f}{\partial x}(x_0, y_0)\mathbf{i} + rac{\partial f}{\partial y}(x_0, y_0)\mathbf{j} ext{ in } 2D.$$

In 3D the gradient vector adds a third component to become

$$\nabla f(x_0, y_0, z_0) = \frac{\partial f}{\partial x}(x_0, y_0, z_0)\mathbf{i} + \frac{\partial f}{\partial y}(x_0, y_0, z_0)\mathbf{j} + \frac{\partial f}{\partial z}(x_0, y_0, z_0)\mathbf{k}.$$

As in one-variable calculus, in the multivariable context differentiation creates a derivative function. However this is now a **vector-valued** function out of a scalar function and a **matrix-valued** function out of a vector-valued function. We will view the function $\nabla f(x, y)$ or $\nabla f(x, y, z)$ as a vector field when we want to visualize its behavior in a domain. Visualizing matrix-valued functions is much harder and might be done by looking at several vector fields simultaneously. Recalling our earlier discussion of dot products in Chapter 1, the gradient vector is usually a row vector when written as a matrix.

The gradient field plot is the higher dimensional analog of the graph of the derivative function in one variable so developing your visual and symbolic understanding of the gradient field is an essential task. Note that we usually drop the word "vector" off the gradient vector field. **Example 3.20** The basic function $f(x, y) = r = \sqrt{x^2 + y^2}$ is the distance from the origin to the point (x, y) so it increases as we move away from the origin. Its gradient vector in components is (x/r, y/r), which is the unit radial field $\mathbf{e_r}$. Thus r has gradient vector $\mathbf{e_r}$. It increases at maximal rate in the radial direction $\mathbf{e_r}$ and the maximal rate of change is of size 1.

The level sets of f(x, y) = r are equally spaced circles and the gradient field, being radial is clearly orthogonal to the circles. The equal spacing tells us the gradient field has constant magnitude.

Example 3.21 $g(x, y) = r^2 = x^2 + y^2$ has gradient in components (2x, 2y) so $\nabla \mathbf{g} = 2\mathbf{r} = 2r\mathbf{e}_r$. Note that the circles $x^2 + y^2 = r^2$ are level sets of both f and g, but with different spacing, which reflects the different magnitudes of the gradient vectors. Note also the factor 2r, which is the derivative of r^2 in the variable r.

In the exercises you will be asked to extend this observation to a general radial function g(r) and relate the gradient to the derivative g'(r).

Here we show the plots of the functions r and r^2 , showing level sets and then gradient fields and finally both level sets and gradients fields together.

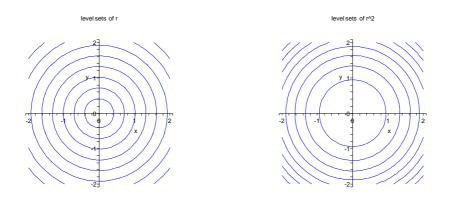


Figure 10: The plots are the level sets of the functions r and r^2 respectively. Notice that the spacing is quite different.

Example 3.22 If $v(x,y) = x^3 + x^2y + xy^2 + y^3$ then $grad(v) = (3x^2 + 2xy + y^2, x^2 + 2xy + 3y^2)$.

Here are plots of the contours and gradient field together for this example, the second in a smaller scale, where the linear approximation starts to be visible (which would be gradient constant, level sets parallel and evenly spaced). In the exercises, you are asked to look on a smaller scale if you have plotting software.

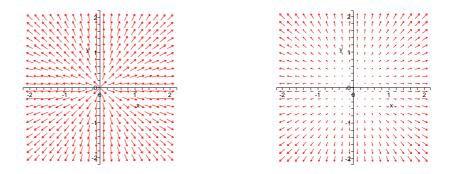


Figure 11: The graphs are of the gradient vector fields for the functions r and r^2 respectively. The vectors are all of length 1 for r (not defined at origin), but scale linearly in size for r^2 .

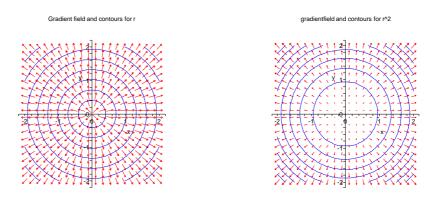


Figure 12: The plots are both the level sets and gradients of the functions r and r^2 respectively. Note how the spacing of level sets is tied to the size of the gradient.

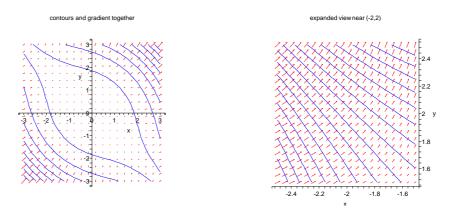


Figure 13: The graphs are of the gradient vector fields and level sets for the polynomial example. The second picture is a smaller scale picture.

3.3.3 Directional derivatives and the gradient

Based on our discussion of linear functions, when we "think locally" we expect to use the gradient vector to find the derivative in any fixed direction. The so-called **directional derivative** measures the instantaneous rate of change for the one-variable function we obtain by only allowing changes in a fixed direction. Graphically we are again slicing the graph, but now with vertical planes not necessarily aligned with the *x* or *y* axis for a function of two variables (functions of three variables are harder to picture, as the graph is in 4D). The result we guess is that for direction vectors **u** the directional derivative of *f* in the direction **u** should be given by the dot product of ∇f with **u**.

A precise definition of directional derivative requires that we express such derivatives as limits, as we did for the special case of partial derivatives in section 3.1. To confirm our conjecture, we mimic the proof in 3.2 about differentiability.

Definition 3.23 The directional derivative of a scalar function f in the direction \mathbf{u} at location \mathbf{r} is denoted by $D_{\mathbf{u}}f(\mathbf{r})$ and is defined to be the following limit:

$$D_{\mathbf{u}}f(\mathbf{r}) = \lim_{h \to 0} \frac{f(\mathbf{r} + h\,\mathbf{u}) - f(\mathbf{r})}{h}$$

To show that $D_{\mathbf{u}}f(\mathbf{r}) = \nabla f \cdot \mathbf{u}$, we do a calculation similar to the proof above in section 3.2 of differentiability assuming continuity of partial derivatives.

Theorem 3.24 Assuming f has continuous partial derivatives in a neighborhood of a location \mathbf{r} , the directional derivative of f in the direction \mathbf{u} at location \mathbf{r} is equal to $\nabla f(\mathbf{r}) \cdot \mathbf{u}$.

Proof: Look at the limit, first in 2D. It has numerator $f(\mathbf{r} + h \mathbf{u}) - f(\mathbf{r})$. As in the proof in section 3.2, pick as intermediate point the point with coordinates given by $\mathbf{r} + h u_1 \mathbf{i}$ where u_1 is the first component of \mathbf{u} , and rewrite the numerator as

$$f(\mathbf{r} + h\,\mathbf{u}) - f(\mathbf{r}) = f(\mathbf{r} + h\,\mathbf{u}) - f(\mathbf{r} + h\,u_1\mathbf{i}) + f(\mathbf{r} + h\,u_1\mathbf{i}) - f(\mathbf{r}).$$

Then the first term involves only a change in the second coordinate, while the second difference involves only a change in first coordinate. Using the mean value theorem, there are points \mathbf{r}_1 and \mathbf{r}_2 so that

$$f(\mathbf{r} + h \mathbf{u}) - f(\mathbf{r} + hu_1 \mathbf{i}) = f_u(\mathbf{r}_1)hu_2, \quad f(\mathbf{r} + hu_1 \mathbf{i}) - f(\mathbf{r}) = f_x(\mathbf{r}_2)hu_1$$

and as $h \to 0$, the points $\mathbf{r_1}$ and $\mathbf{r_2}$ tend to the location \mathbf{r} . After dividing by h and taking the limit, the desired result holds.

Notice that this result implies that the directional derivative is positive if **u** makes an acute angle with ∇f , negative if the angle is obtuse and zero if **u** makes a right angle with ∇f . Recall that linear functions in two or more dimensions have

directions where the function is constant (level sets are in these directions). This extends to general differentiable functions, as we shall see shortly.

Moreover, the above result establishes that **the gradient field of a function is always orthogonal to its level sets**. This follows since in any direction orthogonal to the gradient, we find the directional derivative is zero. Such a directional derivative is related to the derivative of the function along any path, so tangent vectors to paths in the level set will lead to zero directional derivatives. An alternate view of this will be given in the next section using the chain rule.

Differentials notation: In terms of differentials, the change in some direction when infinitesimal will be written as the vector change: $d\mathbf{r}$ and then the change in a function in such a direction becomes:

$$df = \nabla f \cdot d\mathbf{r}.$$

This notation is extremely handy. The differential part appeared in line integrals in Chapter 2 and the Fundamental Theorem for Line Integrals in Chapter 5 will use both the gradient and the differential part.

3.3.4 Important cases: polar and spherical coordinate directions

From the notion of directional derivative, we can specialize to three very important situations: polar coordinates in 2D and spherical and cylindrical coordinates in 3D.

In 2D, the direction of the unit radial vector \mathbf{e}_r is the vector $\cos \theta \mathbf{i} + \sin \theta \mathbf{j}$. Therefore we find the directional derivative in the radial direction to be

$$\nabla f \cdot \mathbf{e}_r = \frac{\partial f}{\partial x} \cos \theta + \frac{\partial f}{\partial y} \sin \theta.$$

Similarly the direction of the unit angular vector \mathbf{e}_{θ} is the vector $-\sin\theta \mathbf{i} + \cos\theta \mathbf{j}$ and the directional derivative becomes:

$$\nabla f \cdot \mathbf{e}_{\theta} = -\frac{\partial f}{\partial x} \sin \theta + \frac{\partial f}{\partial y} \cos \theta.$$

Since these unit direction vectors are everywhere orthogonal, this can be thought of as describing the polar coordinates of the gradient vector field! You might guess that there is another view of the polar coordinate version of the gradient field involving the derivatives in the polar coordinates r and θ . This is the chain rule, described in the next section.

A similar calculation in cylindrical coordinate in 3D expresses the derivatives in the three orthogonal directions found by adding a z dependence. This becomes the

following three relations:

$$\nabla f \cdot \mathbf{e}_r = \frac{\partial f}{\partial x} \cos \theta + \frac{\partial f}{\partial y} \sin \theta$$
$$\nabla f \cdot \mathbf{e}_\theta = -\frac{\partial f}{\partial x} \sin \theta + \frac{\partial f}{\partial y} \cos \theta$$
$$\nabla f \cdot \mathbf{e}_z = \frac{\partial f}{\partial z}.$$

~ ~

In spherical coordinates (ρ, θ, ϕ) , the corresponding formulas relate the gradient in rectangular coordinates (x, y, z) to the spherical ones:

$$\nabla f \cdot \mathbf{e}_{\rho} = \frac{\partial f}{\partial x} \cos \theta \sin \phi + \frac{\partial f}{\partial y} \sin \theta \sin \phi + \frac{\partial f}{\partial z} \cos \phi$$
$$\nabla f \cdot \mathbf{e}_{\theta} = -\frac{\partial f}{\partial x} \sin \theta + \frac{\partial f}{\partial y} \cos \theta$$
$$\nabla f \cdot \mathbf{e}_{\phi} = \frac{\partial f}{\partial x} \cos \theta \cos \phi + \frac{\partial f}{\partial y} \sin \theta \cos \phi - \frac{\partial f}{\partial z} \sin \phi$$

Once we have the chain rule in the next section, we will relate these to derivatives in the cylindrical and spherical variables.

3.3.5 Vector-valued functions and the Jacobian matrix

For a vector valued function \mathbf{v} , written as a column vector with n rows, we get $\mathbf{v}(x, y) - \mathbf{v}(x_0, y_0) \approx \frac{\partial \mathbf{v}}{\partial x}(x_0, y_0) \cdot (x - x_0) + \frac{\partial \mathbf{v}}{\partial y}(x_0, y_0) \cdot (y - y_0)$ as the linear approximation and this creates a **matrix with gradient vectors as the rows**. Letting the components of \mathbf{v} be called v_j the linear approximation for each j is distinct and only involves v_j , leading to a matrix form for the linear approximation:

$$\mathbf{v}(x,y) - \mathbf{v}(x_0,y_0) \approx \begin{pmatrix} \nabla v_1 \\ \nabla v_2 \\ \vdots \\ \nabla v_n \end{pmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix}$$

and as usual a third entry for the z parts in 3D.

Alert readers recognize that this is the same matrix that appeared in the previous section when discussing systems of linear approximation or equivalently systems of differentials.

Example 3.25 Consider the two functions $u(x, y) = x^2 - y^2$ and v(x, y) = 2xy simultaneously, say as a vector with components (u, v). The corresponding Jacobian matrix has rows ∇u and ∇v , which becomes the matrix:

$$\begin{pmatrix} 2x & -2y \\ 2y & 2x \end{pmatrix}$$

This says for approximating changes in u and v simultaneously, use matrix multiplication by this matrix, multiplying changes in x and y.

Note that in this example, the gradients of the two functions are always orthogonal and neither is zero except at the origin in (x, y), so we expect the level sets to be orthogonal even though the functions are clearly non-linear. The level sets form a network of orthogonal hyperbolas, as may be seen in the level set plots below. The second plot is a zoomed-in view near $x = 1, y = \frac{1}{2}$ and shows the local linear behavior.

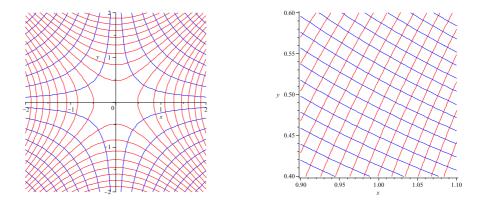


Figure 14: The graphs are of the level sets of $u = x^2 - y^2$ (red) and v = 2xy (blue). The second picture is a smaller scale picture near $(1, \frac{1}{2})$.

Below the level set plots is an attempt to plot the gradient fields simultaneously. It has some defects in terms of our ability to read the pictures.

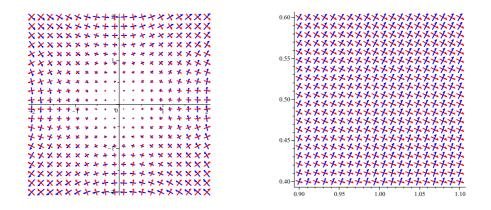


Figure 15: The graphs are of the gradient fields of $u = x^2 - y^2$ (red) and v = 2xy (blue). The second picture is a smaller scale picture near $(1, \frac{1}{2})$.

Notation for the Jacobian: There are a number of ways to denote the Jacobian matrix. Some variations are due to using vectors or naming the components, while others are more substantial and relate also to the distinction between a matrix and the linear mapping it represents in some coordinates, as described briefly in Chapter 1.

The most common notation is the variation of Leibniz notation for a single partial derivative: we write $\frac{\partial(u,v)}{\partial(x,y)}$ for the example above, where u and v are the components in the range and x, y are coordinates in the domain. If the vector **U** has the components (u, v) the vector version of the notation would read: $\frac{\partial \mathbf{U}}{\partial \mathbf{r}}$. This is less common. Other notations would be $D\mathbf{U}, J(u, v; x, y)$ and $d_{(x,y)}\mathbf{U}$.

Warning: Some authors use some of the above for the determinant of the matrix rather than the matrix.

Using the Jacobian: The local behavior of the vector-valued function or a system of several scalar functions considered simultaneously is captured by a Jacobian matrix. Since the rows are the individual gradients, one finds that two rows being proportional at some input value means the level sets near that point are tangential to each other (same linear approximation to level sets). Be aware that the function values may be wildly different (my income, Bill Gates' income) yet have the same linear approximation or related linear approximations proportional in all directions (since I own fewer Microsoft shares than Bill), so we are not saying the graphs are mutually tangent! Changes in the variables are in proportion.

Geometrically, when level sets are not tangent to one another, they form a local grid which locally is formed of parallel pieces. In 2-D, two functions with non-tangent level sets form a grid of parallelograms while in 3-D, two functions form families of planes and it takes three different families to create a coordinate grid (parallelepipeds). This relates to our differentials discussion and our earlier discussion in Chapter 1 about systems of equations: the determinant of the Jacobian describes the signed area or volume of the local level sets!

3.3.6 Some more gradient field plots in 2D and 3D

Gradient fields have a special structure, to be described fully in Chapter 5. For now we content ourselves with practicing computations and viewing plots of gradient fields and level sets. These will be similar to viewing plots of the function and derivative in one variable calculus. Unlike one-variable calculus, we will not typically be plotting the second derivative, since for a scalar function in 3D the second derivative function will be a 3×3 matrix-valued function! Instead, we will be deeply concerned with what information the second derivative conveys, but relate it back to the original function by quadratic approximation, the next level of refinement beyond the linear approximation.

Example 3.26 Consider the function $u(x, y) = \frac{x}{x^2+y^2}$. Find the gradient field and plot it in two scales near (1, 1).

Solution: $\nabla u(x,y) = \frac{y^2 - x^2}{(x^2 + y^2)^2} \mathbf{i} + \frac{-2xy}{(x^2 + y^2)^2} \mathbf{j}$. The gradient fields are plotted below. Note that as we zoom in, the vector field becomes more like a constant vector field, namely $\nabla u(1,1) = -\frac{1}{2}\mathbf{j}$.

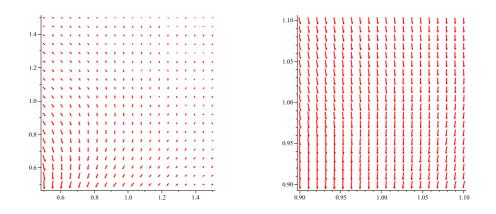


Figure 16: The graphs are of the gradient fields of u near (1,1), with the second plot in a smaller scale.

Example 3.27 Consider the functions $w(x, y, z) = x^2 + y^2 + z^2$ and $\rho(x, y, z) = \sqrt{x^2 + y^2 + z^2}$, and find their gradient fields. Plot the fields and discuss what you see.

Solution: $\nabla w = 2x\mathbf{i} + 2y\mathbf{j} + 2z\mathbf{k} = 2\mathbf{r}$, while $\nabla \rho = \mathbf{r}/\rho = \mathbf{e}_{\rho}$, a unit vector. This is the 3-D version of our earlier discussion. The gradient fields are harder to read in 3-D, but appear below.

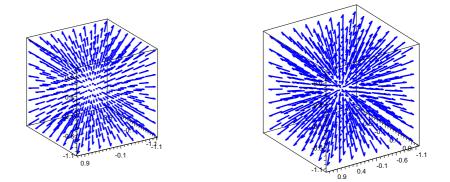


Figure 17: The graphs are of the gradient fields of w and ρ . Note that the magnitude decreases near the origin for w.

3.3.7 EXERCISES

Writing: Explaining, Reacting, Questioning

- 1. Consider two functions f(x, y) and g(x, y). If some level set of f intersects a level set of g at a point (x_0, y_0) , how could you define the angle of intersection using tangent vectors to the level sets? How could you use normal vectors instead? Which one works better for the intersection of f(x, y, z)and g(x, y, z) level sets in 3-D?
- 2. If we are considering the restriction of f(x, y) to a level set of g(x, y) and the point (x_0, y_0) is a local maximum for this restricted function, what can you say about the gradient of f at this point, assuming it exists? In particular, must the gradient be the zero vector there? Recall problem ?? from section 1 which looked along coordinate axes, which is a simple form of g.
- 3. Looking at the components of the 2-D gradient field in the directions e_r and e_{θ} , one would expect to reconstruct the gradient vector using these components. Show that this leads back to the same vector by substitution for the unit vectors e_r and e_{θ} in terms of the usual vectors i and j.
- 4. Consider the function $x^2 y^2$. For the level set $x^2 y^2 = 1$, which consists of two branches of a hyperbola, find the gradient vector, then by solving for y in terms of x and viewing the level set as a graph, confirm that the gradient vector is orthogonal to the level set at every point.
- 5. For the level set $x^2 y^2 = 0$ something different happens at (0, 0). Draw a picture of the level set and describe why the picture would suggest that the gradient is either zero at the origin or does not exist (which is clearly not happening in this example). Formulate your answer as a general principle and then check it for the level sets of $H(x, y) = \frac{1}{2}y^2 + 1 \cos x$, for values H = 0 and H = 2. Level sets of H are important sets in the dynamics of a simple non-linear oscillator (frictionless pendulum).
- 6. Consider a differential equation in the form $\mathbf{r}'(t) = \mathbf{v}(\mathbf{r}(t))$, what condition(s) guarantee that for some scalar function $H(\mathbf{r})$, the composite function $h(t) = H(\mathbf{r}(t))$ is constant as a function of t? Increasing? Decreasing?
- 7. Given a differential equation in the form $\mathbf{r}'(t) = \mathbf{v}(\mathbf{r}(t))$, what condition(s) guarantee that for some scalar function $H(\mathbf{r})$, the composite function $h(t) = H(\mathbf{r}(t))$ is constant as a function of *t*? Increasing? Decreasing?

Calculational Exercises

For problems 1-8 find the gradient vector at the indicated point in the domain:

- 1. $f(x,y) = x^2 y^2$ at (2,4).
- 2. $f(x,y) = y + e^{2x} \cos 3y$ at $(0,\pi)$.

3.
$$f(x,y) = \sin(2x+3y) + 2\cos(2x+3y)$$
 at $(\pi/8,\pi/4)$.
4. $f(x,y) = \frac{1}{x} + \frac{1}{y}$ at $(1,3)$.
5. $g(x,y,z) = \frac{1}{2}\ln(x^2 + y^2 + z^2)$ at $(3,6,6)$.
6. $u(x,y) = \sin 2x e^{-4y}$ at $(\pi/4,1)$.
7. $w(x,y) = \frac{1}{\sqrt{16-x^2-y^2}}$ at $(-1,2)$.
8. $q(x,y) = e^{-x^2-4xy-8y^2}$ at $(-2,-1)$.

For problems 9-16 find the gradient vector field at all points in the domain:

9.
$$f(x, y) = x^4 - 6x^2y^2 + y^4$$

10. $g(x, y) = \cos x \sin y$
11. $u(x, y) = e^{-x^2} \cos y$
12.
13.

14.

15. $\theta(x, y) = \tan^{-1}(y/x)$

16.
$$\phi(x, y, z) = \tan^{-1}(\frac{\sqrt{(x^2 + y^2)}}{z})$$

17. Show that the functions $u(x, y) = x^4 - 6x^2y^2 + y^4$ and $v(x, y) = 4x^3y - 4xy^3$ have orthogonal gradient vectors at all points in the plane.

For problems 25-32, Computer Problems: plot the functions in both domains and describe what happens to the graphs as we zoom in. Do your results suggest the function is differentiable? Why or why not? Remember to watch out for automatic rescaling in the plots.

18.

19.

20.

21.

22.

23.

24.

- 25. For problems 33-42 Computer Problems:
- 26. For problems 25-30, match the listing of gradient plots with the listing of level set plots.