Partial derivatives & Vector calculus

Partial derivatives

Functions of several arguments (multivariate functions) such as f[x,y] can be differentiated with respect to each argument

$$\frac{\partial f}{\partial x} \equiv \partial_x f, \qquad \frac{\partial f}{\partial y} \equiv \partial_y f,$$

etc. One can define higher-order derivatives with respect to the same or different variables

$$\frac{\partial^2 f}{\partial x^2} \equiv \partial_{x,x} f, \qquad \frac{\partial^2 f}{\partial y^2} \equiv \partial_{y,y} f, \qquad \frac{\partial^2 f}{\partial x \, \partial y} \equiv \frac{\partial}{\partial x} \frac{\partial f}{\partial y} \equiv \partial_{x,y} f$$

For most of the functions mixed partial derivatives do not depend on the order of differentiation

$$\frac{\partial^2 f}{\partial x \, \partial y} \equiv \frac{\partial^2 f}{\partial y \, \partial x}$$

This holds if the mixed derivatives are continuous at a given point. For instance,

```
f[x_, y_] = x y;
∂x f[x, y]
∂y f[x, y]
∂y,x f[x, y]
∂x,y f[x, y]

y

x

1

1
```

- **"Bad" functions**

Multivariate series

Taylor series can be generalized for multivariate functions and the

```
f[x_, y_] = Sin[x + y];
Series[f[x, y], {x, 0, 3}]
```

$\mathrm{Sin}[y] + \mathrm{Cos}[y] \, x - \frac{1}{2} \, \mathrm{Sin}[y] \, x^2 - \frac{1}{6} \, \mathrm{Cos}[y] \, x^3 + O[x]^4$

```
Series[f[x, y], {x, 0, 3}, {y, 0, 3}]
```

$\left(y - \frac{y^3}{6} + O[y]^4\right) + \left(1 - \frac{y^2}{2} + O[y]^4\right) x + \left(-\frac{y}{2} + \frac{y^3}{12} + O[y]^4\right) x^2 + \left(-\frac{1}{6} + \frac{y^2}{12} + O[y]^4\right) x^3 + O[x]^4$

or, in the symmetric form

```
Normal[Series[f[x, y], {x, 0, 3}, {y, 0, 3}]]
Expand[Normal[Series[f[x, y], {x, 0, 3}, {y, 0, 3}]]]
```

$$x - \frac{x^3}{6} + \left(1 - \frac{x^2}{2}\right) y + \left(-\frac{x}{2} + \frac{x^3}{12}\right) y^2 + \left(-\frac{1}{6} + \frac{x^2}{12}\right) y^3$$

$$x - \frac{x^3}{6} + y - \frac{x^2 y}{2} - \frac{x y^2}{2} + \frac{x^3 y^2}{12} - \frac{y^3}{6} + \frac{x^2 y^3}{12}$$

Exercise: Find a way to sort this polynomial in increasing powers of x, y.

Vector calculus

Physics makes use of vector differential operations on functions such as *gradient, divergence, curl* (*rotor*), *Laplacian*, etc. In the current version of *Mathematica* realizations of these operations are new and not included in the main body of the software. Instead, these functions are implemented in the optional VectorAnalysis package that has to be called before performing these operations

```
Needs["VectorAnalysis`"]
```

Unfortunately, this package seems to be inconvenient.

- **Gradient**

Gradient of a scalar funtion is a vector defined as

$$\text{grad } f \equiv \nabla f \equiv \mathbf{e}_x \frac{\partial f}{\partial x} + \mathbf{e}_y \frac{\partial f}{\partial y} + \mathbf{e}_z \frac{\partial f}{\partial z} \equiv \left\{\partial_x f, \partial_y f, \partial_z f\right\}$$

One can speak about the gradient operator defined as

$$\nabla \equiv \mathbf{e}_x \frac{\partial}{\partial x} + \mathbf{e}_y \frac{\partial}{\partial y} + \mathbf{e}_z \frac{\partial}{\partial z}$$

that acts on scalar functions of vector arguments. An example of a gradient in physics is force **F** that is minus gradient of the potential energy U[x,y,z] and similar for the electric field **E** that is minus gradient of the electric potential ϕ

$$\mathbf{F} \equiv -\nabla U, \qquad \mathbf{E} \equiv -\nabla \phi$$

Examples trying to use the *Mathematica*'s VectorCalculus package:

Following *Mathematica* help:

```
Clear[x, y, z, U]
U = x² + y² + z²;
Grad[U]
```
```
{0, 0, 0}
```

- a wrong output. An attempt of a standard usage

```
U[x_, y_, z_] = x² + y² + z²;  (* 3d oscillator *)

F[x_, y_, z_] = Grad[U[x, y, z]]
```
```
{0, 0, 0}
```

- same wrong result. Still this command is working with a special naming choice

$$\texttt{Grad}\left[\texttt{Xx}^2 + \texttt{Yy}^2 + \texttt{Zz}^2\right]$$

{2 Xx, 2 Yy, 2 Zz}

However, this naming restriction is inconvenient.

> Fortunately, it is not difficult to program the gradient in *Mathematica*. To use the definition below, quit the kernel to remove the VectorAnalysis package from the memory

In[43]:= $\texttt{Grad[f\_]} := \left\{\partial_x f, \ \partial_y f, \ \partial_z f\right\}$

Since *x,y,z* enters the definition of this function, the arguments of *f* should also be *x,y,z*. With any other notation for the arguments of *f*, it won't work, in contrast to definitions of tru functions.
MyGrad works on expressions

$$\texttt{Grad}\left[\texttt{x}^2 + \texttt{y}^2 + \texttt{z}^2\right] \quad (* \ \nabla\texttt{r}^2 = 2\texttt{r} \ *)$$

{2 x, 2 y, 2 z}

This means

$$\nabla r^2 = 2 \ \mathbf{r}$$

MyGrad also works on functions

```
U[x_, y_, z_] = x² + y² + z²;   (* 3d oscillator *)
V[x_, y_, z_] = x⁴;
Grad[U[x, y, z]]
Grad[V[x, y, z]]
```

{2 x, 2 y, 2 z}

$$\left\{4 \ x^3, \ 0, \ 0\right\}$$

Mathematica has the symbol ∇ but it seems it is only for typing

? ∇

Information::notfound : Symbol ∇ not found. ≫

? E

E is the exponential constant *e* (base of natural logarithms), with numerical value ≃ 2.71828. ≫

$$\texttt{I} == \texttt{i}$$

True

One can define a vector function that is the gradient of a scalar function. For the electric field of a point charge one has

$$\phi[\texttt{x\_, y\_, z\_}] = \frac{\texttt{k Q}}{\sqrt{\texttt{x}^2 + \texttt{y}^2 + \texttt{z}^2}}; \quad (* \ \texttt{Coulomb potential of a point charge} \ *)$$

$$\texttt{EE[x\_, y\_, z\_]} = -\texttt{Grad}[\phi[\texttt{x, y, z}]] \quad (* \ \texttt{Electric field of a point charge} \ *)$$

$$\left\{\frac{\texttt{k Q x}}{\left(\texttt{x}^2 + \texttt{y}^2 + \texttt{z}^2\right)^{3/2}}, \ \frac{\texttt{k Q y}}{\left(\texttt{x}^2 + \texttt{y}^2 + \texttt{z}^2\right)^{3/2}}, \ \frac{\texttt{k Q z}}{\left(\texttt{x}^2 + \texttt{y}^2 + \texttt{z}^2\right)^{3/2}}\right\}$$

Divergence

Divergence of a vector is a scalar defined by

$$\operatorname{div} \mathbf{A} \equiv \nabla \cdot \mathbf{A} \equiv \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$$

divergence can be represented by the operator

$$\nabla \equiv \mathbf{e}_x \frac{\partial}{\partial x} + \mathbf{e}_y \frac{\partial}{\partial y} + \mathbf{e}_z \frac{\partial}{\partial z}$$

same as the gradient operator above. The only difference between them is that gradient acts on scalars and divergence acts on vectors.

In[61]:= `Div[Avec_] := ∂ₓ Avec[[1]] + ∂_y Avec[[2]] + ∂_z Avec[[3]]`

Examples

```
Div[{x, y, z}]
```

```
3
```

```
Fvec[x_, y_, z_] = {x², y², z²};
Div[Fvec[x, y, z]]
```

```
2 x + 2 y + 2 z
```

```
Fvec[x_, y_, z_] = {y, x, x y};
Div[Fvec[x, y, z]]
```

```
0
```

■ Laplacian

Laplacian is a second-order vector differential operation. Laplacian of a scalar f is defined as div grad f and denoted by Δ or ∇^2

$$\Delta f \equiv \operatorname{div} \operatorname{grad} f \equiv \nabla \cdot \nabla f \equiv \nabla^2 f$$

From this definition follows

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

The Laplace operator

$$\Delta \equiv \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

can be obtained by squaring the gradient / divergence operator above.

`Laplace[f_] := ∂_{x,x} f + ∂_{y,y} f + ∂_{z,z} f`

Example

```
f[x_, y_, z_] = x² + y² + z²;
Laplace[f[x, y, z]]
```

6

Laplacian of a vector is defined in components through Laplacians of the components as

$$\triangle \mathbf{A} \equiv \mathbf{e}_1 \triangle A_1 + \mathbf{e}_2 \triangle A_2 + \mathbf{e}_3 \triangle A_3$$

In[60]:=
```
LaplaceVec[Avec_] := {∂ₓ,ₓAvec[[1]] + ∂ᵧ,ᵧAvec[[1]] + ∂_z,zAvec[[1]],
   ∂ₓ,ₓAvec[[2]] + ∂ᵧ,ᵧAvec[[2]] + ∂_z,zAvec[[2]],
   ∂ₓ,ₓAvec[[3]] + ∂ᵧ,ᵧAvec[[3]] + ∂_z,zAvec[[3]]}
```

■ Curl (rotor)

Curl of a vector is a vector defined by

$$\mathrm{curl}\ \mathbf{A} \equiv \det \left[\begin{pmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ \partial_x & \partial_y & \partial_z \\ A_x & A_y & A_z \end{pmatrix} \right] \equiv \nabla \times \mathbf{A}$$

In[62]:=
```
Curl[Avec_] :=
   {∂ᵧAvec[[3]] - ∂_zAvec[[2]], ∂_zAvec[[1]] - ∂ₓAvec[[3]], ∂ₓAvec[[2]] - ∂ᵧAvec[[1]]}
```

Examples

```
Curl[{x, y, z}]
```

{0, 0, 0}

```
Curl[{y, -x, 0}]
```

{0, 0, -2}

■ Repeated first-order differential vector operations

Repeated vector differential operations satisfy some identities that are similar to repeated vector products if one uses the ∇ operator and considers it as a vector.

■ Double curl

Similarly to the double vector product $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) \equiv \mathbf{B}\ (\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}\ (\mathbf{A} \cdot \mathbf{B})$, one has

$$\mathrm{curl}\ \mathrm{curl}\ \mathbf{A} \equiv \nabla \times (\nabla \times \mathbf{A}) \equiv \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} \equiv \mathrm{grad}\ (\mathrm{div}\ \mathbf{A}) - \triangle \mathbf{A}$$

Note that here the vector A is always rightmost because the differential operators are acting on it. Check this identity

```
Avec[x_, y_, z_] = {Avecx[x, y, z], Avecy[x, y, z], Avecz[x, y, z]};
```

```
Curl[Curl[Avec[x, y, z]]]
```

$\{-\mathrm{Avecx}^{(0,0,2)}[x, y, z] - \mathrm{Avecx}^{(0,2,0)}[x, y, z] + \mathrm{Avecz}^{(1,0,1)}[x, y, z] + \mathrm{Avecy}^{(1,1,0)}[x, y, z],$
  $-\mathrm{Avecy}^{(0,0,2)}[x, y, z] + \mathrm{Avecz}^{(0,1,1)}[x, y, z] + \mathrm{Avecx}^{(1,1,0)}[x, y, z] - \mathrm{Avecy}^{(2,0,0)}[x, y, z],$
  $\mathrm{Avecy}^{(0,1,1)}[x, y, z] - \mathrm{Avecz}^{(0,2,0)}[x, y, z] + \mathrm{Avecx}^{(1,0,1)}[x, y, z] - \mathrm{Avecz}^{(2,0,0)}[x, y, z]\}$

```
Grad[Div[Avec[x, y, z]]]
```

$\{$Avecz$^{(1,0,1)}$[x, y, z] + Avecy$^{(1,1,0)}$[x, y, z] + Avecx$^{(2,0,0)}$[x, y, z],
 Avecz$^{(0,1,1)}$[x, y, z] + Avecy$^{(0,2,0)}$[x, y, z] + Avecx$^{(1,1,0)}$[x, y, z],
 Avecz$^{(0,0,2)}$[x, y, z] + Avecy$^{(0,1,1)}$[x, y, z] + Avecx$^{(1,0,1)}$[x, y, z]$\}$

```
LaplaceVec[Avec[x, y, z]]
```

$\{$Avecx$^{(0,0,2)}$[x, y, z] + Avecx$^{(0,2,0)}$[x, y, z] + Avecx$^{(2,0,0)}$[x, y, z],
 Avecy$^{(0,0,2)}$[x, y, z] + Avecy$^{(0,2,0)}$[x, y, z] + Avecy$^{(2,0,0)}$[x, y, z],
 Avecz$^{(0,0,2)}$[x, y, z] + Avecz$^{(0,2,0)}$[x, y, z] + Avecz$^{(2,0,0)}$[x, y, z]$\}$

```
Curl[Curl[Avec[x, y, z]]] == Grad[Div[Avec[x, y, z]]] - LaplaceVec[Avec[x, y, z]]
```

True

- **Divergence of a curl**

(of a solenoidal field) is zero

$$\operatorname{div} \operatorname{curl} \mathbf{A} \equiv \nabla \cdot (\nabla \times \mathbf{A}) \equiv 0$$

Check this identity

```
Div[Curl[Avec[x, y, z]]]
```

0

- **Curl of a gradient**

(of a potential field) is also zero

$$\operatorname{curl} \operatorname{grad} f \equiv \nabla \times (\nabla f) \equiv 0$$

Check this identity

```
Curl[Grad[f]]
```

{0, 0, 0}

- **Gradient of a divergence**

This one seems to be not expressible via other operations

$$\operatorname{grad} \operatorname{div} \mathbf{A} \equiv \nabla (\nabla \cdot \mathbf{A}) \equiv ?$$

```
Grad[Div[Avec[x, y, z]]]
```

$\{$Avecz$^{(1,0,1)}$[x, y, z] + Avecy$^{(1,1,0)}$[x, y, z] + Avecx$^{(2,0,0)}$[x, y, z],
 Avecz$^{(0,1,1)}$[x, y, z] + Avecy$^{(0,2,0)}$[x, y, z] + Avecx$^{(1,1,0)}$[x, y, z],
 Avecz$^{(0,0,2)}$[x, y, z] + Avecy$^{(0,1,1)}$[x, y, z] + Avecx$^{(1,0,1)}$[x, y, z]$\}$

- **Differential vector operations on two objects**

- **Gradient of a product of two scalars**

$$\operatorname{grad} (\phi \, \psi) \equiv \nabla (\phi \, \psi) \equiv \phi \, \nabla \psi + \psi \, \nabla \phi$$

Check this identity

```
Grad[ϕ[x, y, z] ψ[x, y, z]] == ϕ[x, y, z] Grad[ψ[x, y, z]] + Grad[ϕ[x, y, z]] ψ[x, y, z]
```
```
True
```

- **Divergence and curl of a product of a vector and a scalar**

    ```
    div (ϕ A) ≡ ∇ · (ϕ A) ≡ ϕ ∇ · A + ∇ϕ · A
    curl (ϕ A) ≡ ∇ × (ϕ A) ≡ ϕ ∇ × A + ∇ϕ × A
    ```

Check these identities

- **Divergence of a vector product**

    ```
    div (A × B) ≡ ∇ · (A × B) ≡ (∇ × A) · B − A · (∇ × B)
    ```

Check this identity

```
Avec[x_, y_, z_] = {Avecx[x, y, z], Avecy[x, y, z], Avecz[x, y, z]};
Bvec[x_, y_, z_] = {Bvecx[x, y, z], Bvecy[x, y, z], Bvecz[x, y, z]};
Simplify[
 Div[Cross[Avec[x, y, z], Bvec[x, y, z]]] ==
   Curl[Avec[x, y, z]].Bvec[x, y, z] - Avec[x, y, z].Curl[Bvec[x, y, z]]
]
```
```
True
```

Potential and its gradient

Force and electric field are negative gradients of the potential energy and electric potential, respectively:

$$\mathbf{F} \equiv -\nabla U, \qquad \mathbf{E} \equiv -\nabla\phi.$$

Gradient is perpendicular to the equipotential lines and it shows the direction of the strongest increase of the potential. (Thus the force shows the direction of the strongest decrease of the potential. This is natural because all systems tend to decrease their energy and the forces are developed accordingly to this). To prove this, consider an equipotential surface

```
U[x, y, z] = U₀
```

that goes through the point $\mathbf{r}_0 = \{x_0, y_0, z_0\}$. Expanding the potential around $\mathbf{r}_0$ up to the first order, one obtains

$$U[x, y, z] = U_0 + U'_x (x - x_0) + U'_y (y - y_0) + U'_z (z - z_0).$$

Together with the preceding formula this yields the equation of the plane tangential to the equipotential surface at $\mathbf{r}_0$

$$U'_x (x - x_0) + U'_y (y - y_0) + U'_z (z - z_0) = 0,$$

where $V'_\alpha \equiv \partial_\alpha V$. Any vector $\mathbf{r}$ within this plane can be represented in the form

$$\mathbf{r} = \mathbf{r}_0 + \rho,$$

where

$$\rho = \mathbf{e}_x (x - x_0) + \mathbf{e}_y (y - y_0) + \mathbf{e}_z (z - z_0).$$

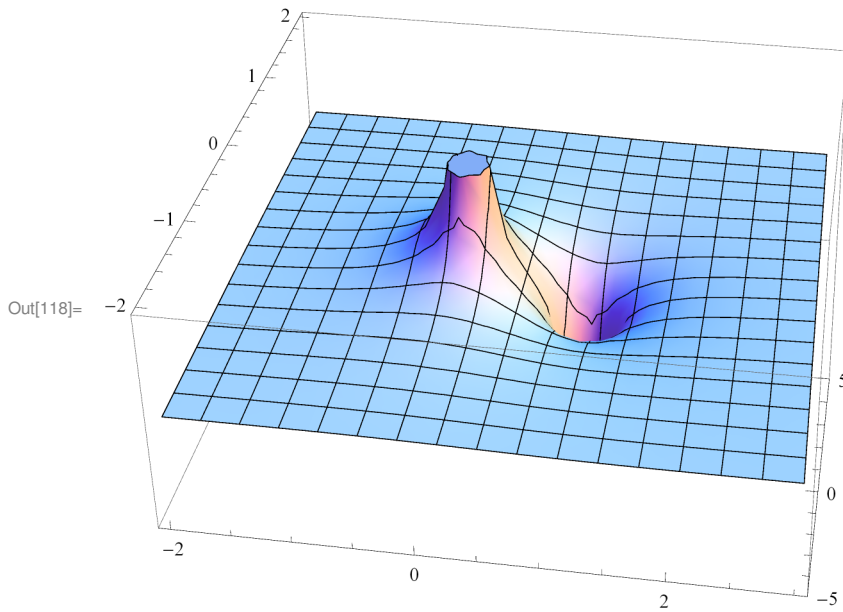One can see that ρ is perpendicular to the gradient because

$$\rho \cdot \nabla U = \left(\mathbf{e}_x (x - x_0) + \mathbf{e}_y (y - y_0) + \mathbf{e}_z (z - z_0)\right) \cdot \left(\mathbf{e}_x U'_x + \mathbf{e}_y U'_y + \mathbf{e}_z U'_z\right)$$
$$= U'_x (x - x_0) + U'_y (y - y_0) + U'_z (z - z_0) = 0.$$

As an example consider the electric potential created by two charges put at (0,0,0) and (a,0,0). In the (x,y) plane (z=0) the potential has the form
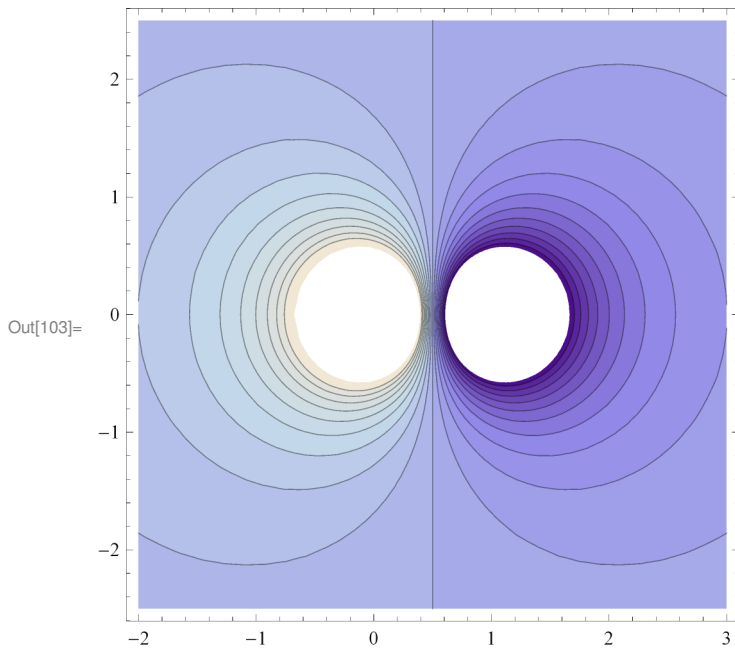
In[116]:= `Q₁ = 1; Q₂ = -1; a = 1;`

$$V[x\_, y\_] = \frac{Q_1}{\left(x^2 + y^2\right)^{1/2}} + \frac{Q_2}{\left(\left(x - a\right)^2 + y^2\right)^{1/2}};$$

`Plot3D[V[x, y], {x, -2, 2 + a}, {y, -2, 2}, PlotRange → {-5, 5}]`

Out[118]=

In[103]:= `EquipotentialLines = ContourPlot[V[x, y], {x, -2, 2 + a}, {y, -2.5, 2.5}, Contours → 20]`

Out[103]=

The electric field in the (x,y) plane is given by.
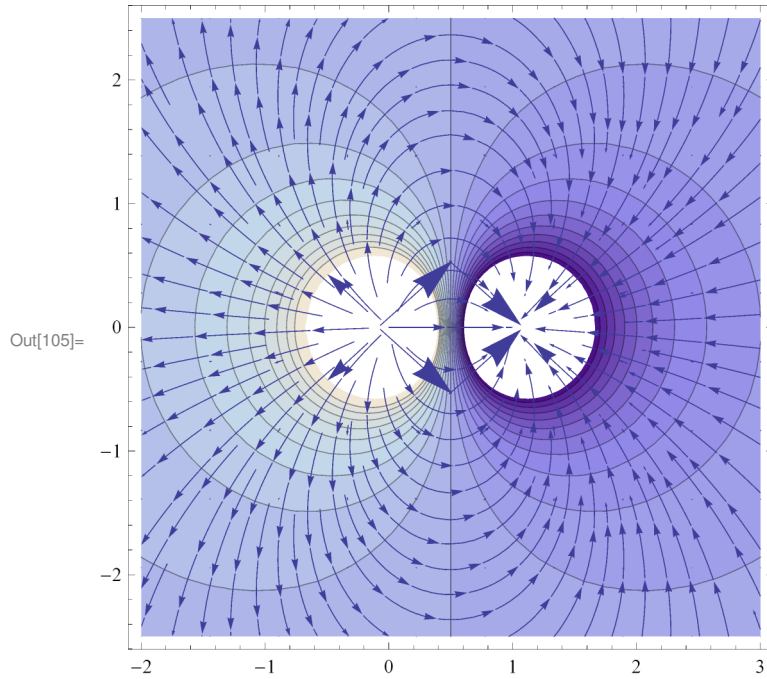
In[44]:= `EE[x_, y_] = -Grad[V[x, y]]`

Out[44]= $\left\{ -\frac{-1 + x}{\left(\left(-1 + x\right)^2 + y^2\right)^{3/2}} + \frac{x}{\left(x^2 + y^2\right)^{3/2}}, -\frac{y}{\left(\left(-1 + x\right)^2 + y^2\right)^{3/2}} + \frac{y}{\left(x^2 + y^2\right)^{3/2}}, 0 \right\}$

Lines of the electric field are shown in the StreamPlot where we plot only x- and y-components

In[106]:= `LinesE = StreamPlot[{EE[x, y][[1]], EE[x, y][[2]]},`
      `{x, -2, 2 + a}, {y, -2.5, 2.5}, VectorPoints → 10];`

Combine the two plots

In[105]:= `Show[EquipotentialLines, LinesE]`

Out[105]=

Lines of electric field should be perpendicular to the equipotential lines because they show the direction of the strongest decrease of the electric potential. However, it seems that Mathematica is not sufficiently precise in plotting to see it.