# TO SMOOTH OR NOT TO SMOOTH
## a note on two-step numerical modeling

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## OBJECTIVE

The purpose of this note is to gain insight in some basic properties of the two-step numerical modeling approach, which consists of an artificial smoothing/regularization step followed by an error-consistent discretization step, cf. Figure 1. We do this by studying its behavior for the simple model problem of finding a reliable numerical approximation of a given non-smooth function, using a constant smoothing coefficient and a uniform grid. We present and analyze both the numerical scheme that is used and the results that are obtained.

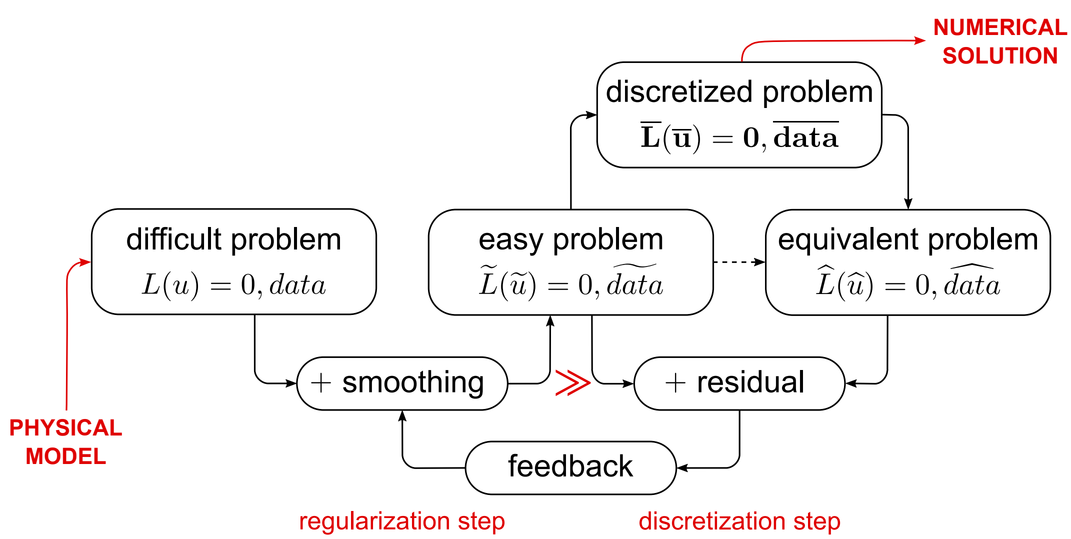


**FIG. 1. The two-step numerical modeling approach**

## THE MODEL PROBLEM

The problem that we consider is:

$$u(x) = f(x) \ , \tag{1}$$

with function $f(x)$ given, and an approximation of 'unknown' solution $u(x)$ to be determined numerically. Because we want to investigate basic modeling principles, the given function is taken equal to:

$$f(x) = \begin{cases} 0 \ , \ x < x_{\mathrm{c}} \ , \\ 1 \ , \ x > x_{\mathrm{c}} \ . \end{cases} \tag{2}$$

A simple piecewise constant function has been chosen to allow us to concentrate on a single numerical difficulty. With (2), the only numerical problem is finding a suitable discrete approximation of the discontinuity.

## TWO-STEP NUMERICAL MODELING

We do not discretize (1) directly, but first add an artificial smoothing/regularization term, i.e., instead of trying to find an approximation for non-smooth $u$ directly by solving 'difficult' problem (1), we propose to solve the 'easy' problem:

$$\widetilde{u}(x) - \frac{d}{dx}\left(\nu_{\mathrm{art}}\frac{d\widetilde{u}}{dx}\right) = f(x) \ , \tag{3}$$

with $\nu_{\mathrm{art}} \geq 0$ the constant artificial smoothing coefficient. For later reference, the equation has been written in a form that is also valid for variable $\nu_{\mathrm{art}}$.

The exact, smooth solution of (3) with $f$ as in (2) reads:

$$\widetilde{u}(x) = \begin{cases} \frac{1}{2}\exp\left(\frac{x - x_{\mathrm{c}}}{\sqrt{\nu_{\mathrm{art}}}}\right) \ , \ x \leq x_{\mathrm{c}} \ , \\ 1 - \frac{1}{2}\exp\left(-\frac{x - x_{\mathrm{c}}}{\sqrt{\nu_{\mathrm{art}}}}\right) \ , \ x \geq x_{\mathrm{c}} \ . \end{cases} \tag{4}$$

We now introduce a uniform grid, with grid points $x_j$ satisfying $x_j - x_{j-1} = \Delta x$, where $\Delta x$ is the constant size of the grid cells. Smooth solution $\widetilde{u}$ of (3) will be numerically approximated on this grid by the piecewise linear, discrete function:

$$\overline{u}(x) = \frac{x_j - x}{\Delta x}u_{j-1} + \frac{x - x_{j-1}}{\Delta x}u_j \ , \ x_{j-1} \leq x \leq x_j \ , \ \forall j \ , \tag{5}$$

with $u_j$ the grid point values of $\overline{u}$.

The accuracy that can be attained with approximation (5) depends on the smoothness of $\widetilde{u}$ with respect to the grid, i.e., on the value of the artificial smoothing coefficient and the size of the grid. By taking $\nu_{\mathrm{art}}$ sufficiently large and $\Delta x$ sufficiently small, *discretization errors* can be kept very small. Obviously, to keep *smoothing errors* small a small value of $\nu_{\mathrm{art}}$ is required, so a small *total numerical error* (i.e., a small difference between $u$ and $\overline{u}$) can only be obtained if a fine grid is used.

An error-consistent discretization of (3) is obtained by integrating this equation over finite volumes, replacing $\widetilde{u}$ by its approximation $\overline{u}$. The boundaries of these finite volumes are formed by the cell centers $\frac{1}{2}(x_{j-1} + x_j)$, which will be denoted by $x_{j-\frac{1}{2}}$. A discretization is then obtained, not just for this problem but for advection-diffusion-reaction-type equations discretized on (moving) curvilinear grids in general, where all leading second-order discretization errors in the equations can be shown to scale with the leading piecewise linear interpolation errors in the variables, cf. (Borsboom 1998; Borsboom 2001; Borsboom 2002; Borsboom 2021) (only 1D analyses; extension to multi-D has been shown to be possible). Smoothness is required to ensure that these leading errors are the dominant discretization errors. Structured grids are required to allow the construction of sufficiently smooth and differentiable close approximations (the equivalent functions) to all discrete function approximations (which by the way includes the coordinate transformation defined by the grid) in a global computational space with uniform Cartesian grid, to allow the assessment of these dominant discretization/interpolation errors.

By making the smoothing/regularization a proper function of the dominant interpolation errors (the feedback loop in Figure 1), it is ensured that the smoothing errors in the first step will always be dominant over all discretization errors in the second step, guaranteeing that the numerical modeling error predominantly consists of physically interpretable smoothing errors. Since the smoothing is a *known* function of gridsize-dependent discretization/interpolation errors, it can be reduced/minimized by a proper redesign of the grid. Notice that in this way *only* numerical errors are reduced/minimized. Physical modeling errors in model equations and data remain unchanged. The development of something like an automatic error-minimizing grid adaptation procedure is therefore not worth the effort if such a procedure will predominantly refine grids (and reduce numerical errors) in areas with large physical modeling errors, which is more than likely to occur in typical shallow-water applications. Large local grid refinements will primarily occur in regions of steep gradients where physical models tend to be anything but reliable. Think of steep gradients/variations in the bathymetry or of discontinuous hydraulic jumps, both violating the shallow-water assumptions, or of steep gradients/variations in the boundary layer at bottom and side walls where the validity of the applied physical models (turbulence model, bed shear-stress model) tend to be limited, especially in the case of varying conditions (non-uniform/undulating surfaces, accelerating/decelerating flow, variable roughness, ...) that may even be partially or fully unknown. The situation This does not apply if it would be possible to take physical error sources into account in the automatic grid optimization procedure.

The error-consistent discretization of (3) on a uniform grid of size $\Delta x$ using discrete function approximation (5) reads:

$$\Big(\frac{\Delta x}{8}-\frac{\nu_{\rm art}}{\Delta x}\Big)u_{j-1}+\Big(\frac{3\Delta x}{4}+2\frac{\nu_{\rm art}}{\Delta x}\Big)u_j+\Big(\frac{\Delta x}{8}-\frac{\nu_{\rm art}}{\Delta x}\Big)u_{j+1}=\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}}f(x)\,dx\;. \qquad (6)$$

Notice the mass matrix $(\frac{1}{8},\frac{3}{4},\frac{1}{8})$, which results from integrating a piecewise linear function over the indicated finite volumes. We will see later that because of this mass matrix, discretization (6) turns out to have a number of desirable properties.

Equation (6) with $f$ as in (2) can be solved exactly as well. Denoting the index of the finite volume that contains the discontinuity by $j_{\rm c}$ (i.e., $x_{j_{\rm c}-\frac{1}{2}}\le x_{\rm c}<x_{j_{\rm c}+\frac{1}{2}}$), the

solution is:

$$u_j = \begin{cases} \beta^{(j_c - j)}\, u_{j_c}\ ,\ j < j_c\ , \\ \dfrac{1}{2} - \delta_c \dfrac{1-\beta}{1+\beta}\ ,\ j = j_c\ , \\ 1 - \beta^{(j-j_c)}\,(1 - u_{j_c})\ ,\ j > j_c\ , \end{cases} \tag{7}$$

with:

$$\beta = \begin{cases} 1 + \dfrac{\frac{1}{2}}{\alpha - \frac{1}{8}} + \sqrt{\left(1 + \dfrac{\frac{1}{2}}{\alpha - \frac{1}{8}}\right)^2 - 1}\ ,\ \alpha < \dfrac{1}{8}\ , \\ 0\ ,\ \alpha = \dfrac{1}{8}\ , \\ 1 + \dfrac{\frac{1}{2}}{\alpha - \frac{1}{8}} - \sqrt{\left(1 + \dfrac{\frac{1}{2}}{\alpha - \frac{1}{8}}\right)^2 - 1}\ ,\ \alpha > \dfrac{1}{8}\ , \end{cases} \tag{8}$$

and:

$$\delta_c = \frac{x_c - x_{j_c}}{\Delta x}\ . \tag{9}$$

The special form of expression (8) is required to avoid the singularity at $\alpha = \frac{1}{8}$. It is easy to verify that $|\beta| < 1$ for any value of $\alpha \geq 0$, i.e., left and right of the discontinuity at $x_c$, the numerical approximation $\overline{u}(x)$ of the solution of (3) converges exponentially to the value 0 and 1 of the exact solution $u(x)$ of (1), just like the exact solution $\widetilde{u}(x)$ of (3) that was given in (4). It is also easy to verify that $\beta$ is a continuous function of $\alpha$. From (7) it then follows that the grid point values $u_j$ depend continuously on $\alpha$ as well. The form of discretization (6) already suggested this property.

For $\alpha < \frac{1}{8}$ we have $\beta < 0$, i.e., a value of $\alpha \geq \frac{1}{8}$ must be used to obtain a non-oscillating numerical solution. Notice that this only applies in the vicinity of steep gradients; in regions where the solution is smooth, a value of $\alpha \ll \frac{1}{8}$ can be used, and should be used to ensure maximum numerical accuracy. Obviously, if both requirements are to be met, an $\alpha$ that varies in space must be used.

The parameter $\delta_c$ defined in (9) indicates the position of the discontinuity relative to the grid. From $x_{j_c - \frac{1}{2}} \leq x_c < x_{j_c + \frac{1}{2}}$ we obtain $\delta_c \in [-\frac{1}{2}, \frac{1}{2})$. Because of the symmetry of the problem, it is sufficient to consider only the values of $\delta_c$ in the range $-\frac{1}{2} \leq \delta_c \leq 0$.

By solving discretized problem (6) we do not solve (3), but an equivalent problem involving an approximation of (3). This equivalent equation, which is a differential equation, cannot be obtained in explicit form if we consider piecewise linear function $\overline{u}$ directly, because higher derivatives of $\overline{u}$ are not defined. To enable an a posteriori error analysis, we therefore define the smooth, infinitely differentiable, and very close approximation $\widehat{u}$ of $\overline{u}$. It is always possible to construct such a function, especially if $\overline{u}$ is fairly regular, i.e., if the (relative) change of the piecewise constant slope of $\overline{u}$ across grid points is not too large.

Equivalent solution $\widehat{u}$ is not uniquely defined; there are several ways to construct it. The most obvious choice is to define a smooth function that passes through the grid point values $u_j$, in which case we have $\widehat{u}(x_j) = u_j = \overline{u}(x_j)$. But we may just as well construct a function that passes through the cell center values[1], satisfying $\widehat{u}(x_{j-\frac{1}{2}}) = \overline{u}(x_{j-\frac{1}{2}}) = \frac{1}{2}(u_{j-1} + u_j)$. This suggests to consider the one-parameter family of equivalent solutions that is obtained by interpolating linearly between a smooth approximation through the grid point values ($\gamma = 0$), and one through the cell center values ($\gamma = 1$).

The value of $\gamma$ that gives the closest smooth approximation depends on the form of $\overline{u}$ (smooth, very smooth, not so smooth, inflection point), and on the details of the construction of $\widehat{u}$. In general, it is obtained for $\gamma \approx \frac{2}{3}$. Fortunately, these details are quite irrelevant. The only thing that matters is to know that it is possible to construct a function $\widehat{u}$ satisfying the requirements: it should be a smooth, infinitely differentiable, and close approximation of $\overline{u}$. These requirements can all be met if $\overline{u}$ is sufficiently regular.

From an error analysis we obtain that by applying (6), we solve, instead of (3), the equivalent differential equation (Borsboom 1998; Borsboom 2002):

$$\big(\widehat{u} + \gamma_0 D_x(\widehat{u})\big) - \nu_{\text{art}} \frac{d^2}{dx^2} \big(\widehat{u} + \gamma_2 D_x(\widehat{u})\big) = f + O(\Delta x^4) \; , \tag{10}$$

with:

$$\gamma_0 = \frac{2 - 3\gamma}{24} \; , \tag{11}$$

$$\gamma_2 = \frac{1 - 3\gamma}{24} \; , \tag{12}$$

$$D_x = \Delta x^2 \frac{d^2}{dx^2} \; , \tag{13}$$

and $\gamma$ the parameter ($\geq 0, \leq 1$) that defines how smooth approximation $\widehat{u}$ is obtained from the grid point values of $\overline{u}$.

## NUMERICAL EXPERIMENTS

To illustrate the behavior of the two-step method, we show results for four positions of the discontinuity relative to the grid:

- $\delta_c = (x_c - x_{j_c})/\Delta x = 0$ (discontinuity at grid point),
- $\delta_c = (x_c - x_{j_c})/\Delta x = -1/2$ (discontinuity at cell center),
- $\delta_c = (x_c - x_{j_c})/\Delta x = -1/4$ (discontinuity in between grid point and cell center),
- $\delta_c = (x_c - x_{j_c})/\Delta x = -3/8$ (discontinuity at position where numerical approximation gives smallest discretization error, see below).

[1]Note that we may also define a function $\widehat{u}$ that passes through both sets of values. Such a function can still be infinitely differentiable, and will indeed be a very close approximation of $\overline{u}$. It will, however, not be a very smooth function. If grid point values as well as cell center values are used, the piecewise constant, and hence discontinuous derivative of piecewise linear $\overline{u}$ is to some extent copied to $\widehat{u}$, leading to spurious inflection points within grid cells. The artificial creation of such meaningless details at subgrid level can only be avoided if for the construction of $\widehat{u}$ at most one value of $\overline{u}$ per grid cell is used. On the other hand, to obtain the closest possible approximation, the largest possible number of values of $\overline{u}$ must be used. In consequence, smooth fit $\widehat{u}$ must be based on exactly one value of $\overline{u}$ per grid cell.

We show:

- exact solution $u$ of (1), i.e., given function (2),
- smooth solution $\widetilde{u}$ of (3), i.e., function (4),
- numerical solution $\overline{u}$ as specified in (5), with grid point values $u_j$ determined by solution of (6), which is given in (7),
- two smooth approximations $\widehat{u}$ of $\overline{u}$, one through the grid point values of $\overline{u}$ ($\gamma = 0$) and one through the cell center values ($\gamma = 1$).

The approximations of $u$ (i.e., $\widetilde{u}$, $\overline{u}$, and the two $\widehat{u}$) are given for two values of the artificial smoothing coefficient:

- $\alpha = \nu_{\rm art}/\Delta x^2 = 1/8$ (value for which (6) gives the closest approximation to the solution of (1)),
- $\alpha = \nu_{\rm art}/\Delta x^2 = 2$ (typical example of a reasonable amount of smoothing).

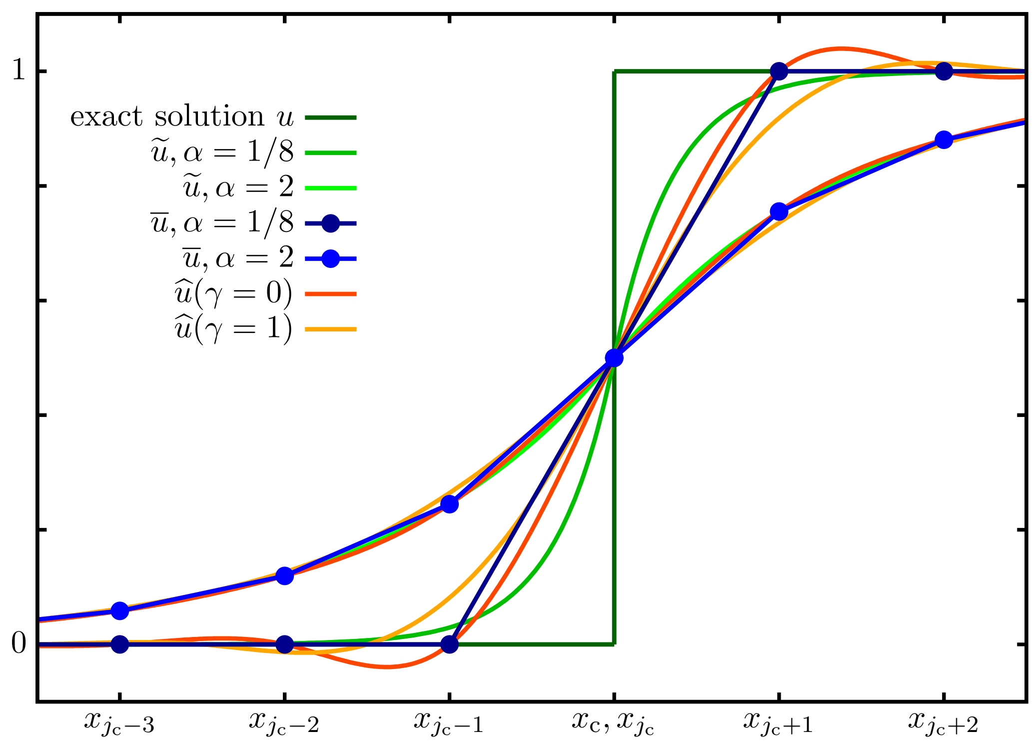


**FIG. 2. Discontinuity at grid point ($\delta_c = 0$)**

The choice $\alpha = \frac{1}{8}$ leads to numerical approximations that, although close to the exact solution, depend considerably on the position of the discontinuity. With $\alpha = \frac{1}{8}$, the numerical solution is spread over two grid cells when the discontinuity is at a grid point (Figure 2), but over only one cell when it is at a cell center (Figure 3). For these two positions the numerical solution obtained is symmetric, but in general it is highly asymmetric for low values of $\alpha$. From (5), (7), and (9) we obtain, for the range

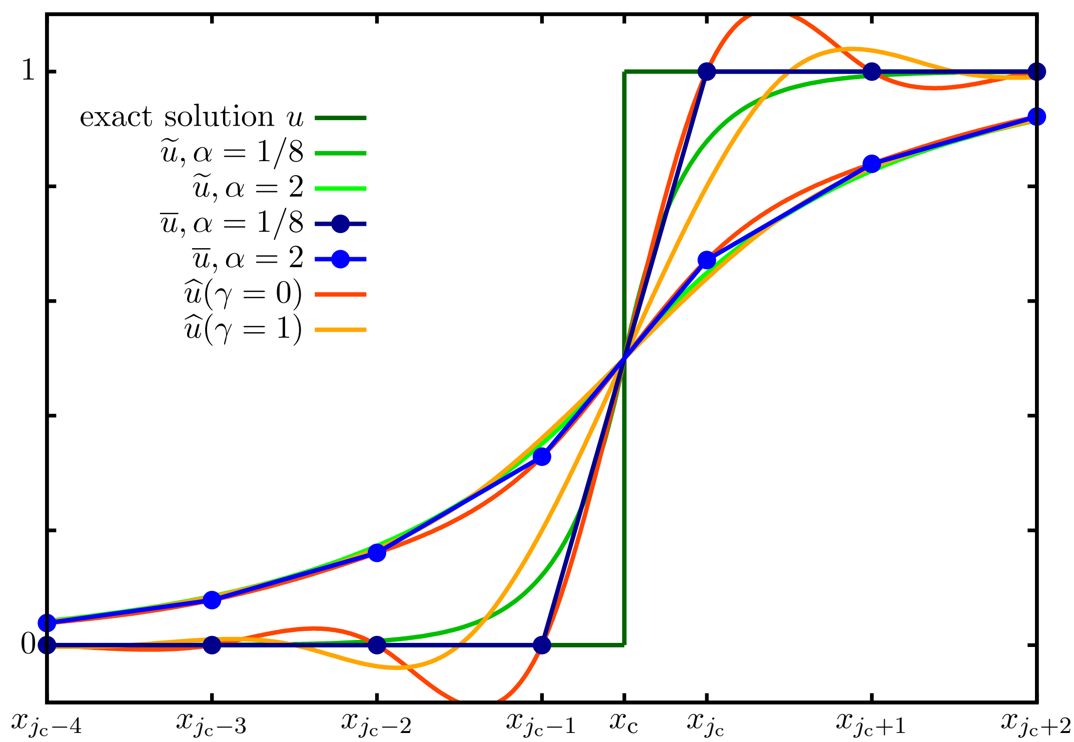


**FIG. 3. Discontinuity at cell center ($\delta_c = -1/2$)**

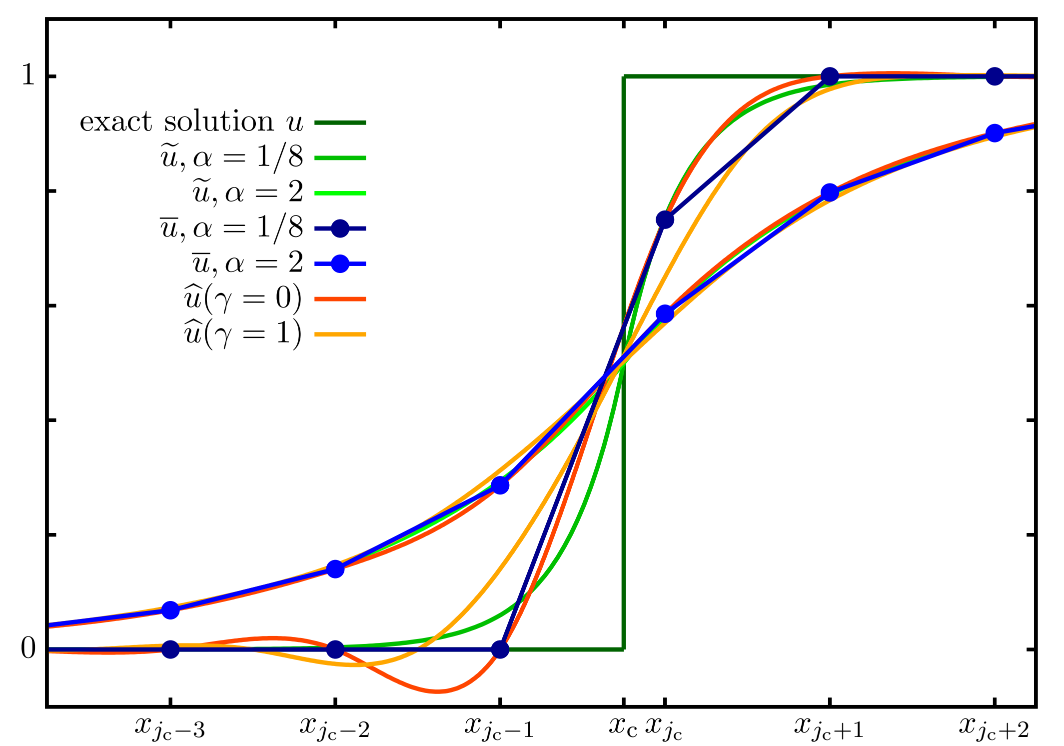


**FIG. 4. Discontinuity in between grid point and cell center ($\delta_c = -1/4$)**

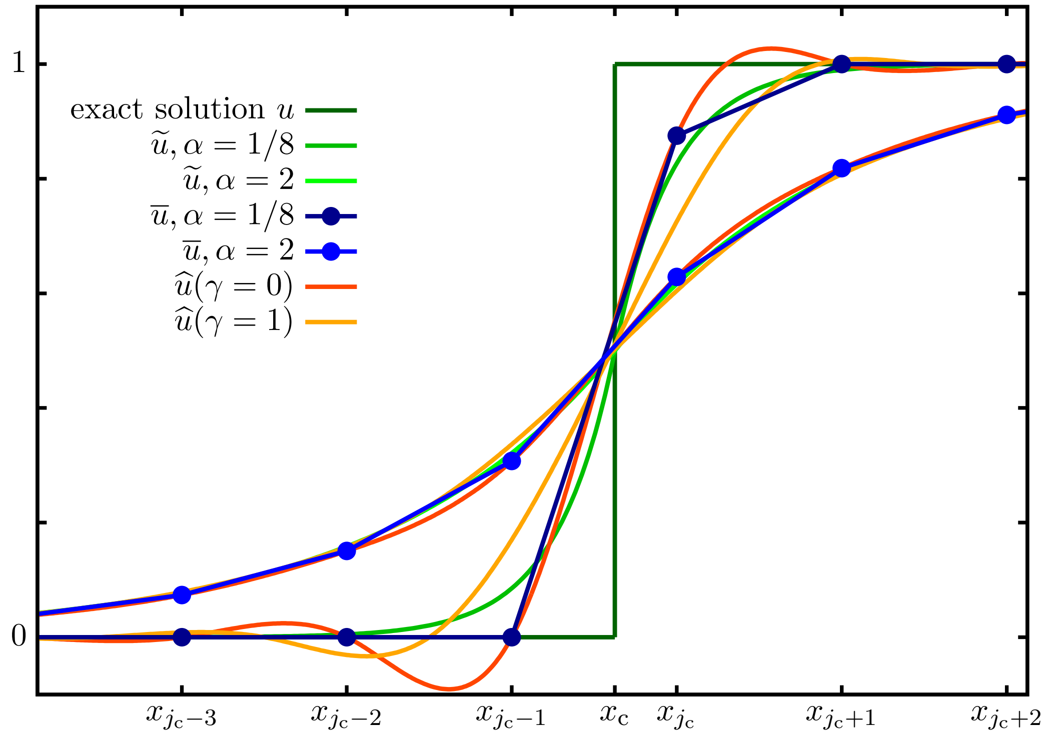


**FIG. 5. Discontinuity with smallest discretization error ($\delta_c = -3/8$)**

$\delta_c \in [-\frac{1}{2}, 0]$ that we consider:

$$\begin{aligned}\overline{u}(x_c) &= \frac{x_{j_c} - x_c}{\Delta x} u_{j_c-1} + \frac{x_c - x_{j_c-1}}{\Delta x} u_{j_c} = -\delta_c u_{j_c-1} + (\delta_c + 1) u_{j_c} \\ &= \Big(1 + \delta_c(1-\beta)\Big)\left(\frac{1}{2} - \delta_c \frac{1-\beta}{1+\beta}\right), \; -\frac{1}{2} \le \delta_c \le 0 \, .\end{aligned} \tag{14}$$

It follows that for $\alpha = \frac{1}{8}$ and hence $\beta = 0$ (cf. (8)) we have $\overline{u}(x_c) = \frac{1}{2} - \delta_c(\frac{1}{2} + \delta_c)$. As expected, this is only equal to $\frac{1}{2}$ for $\delta_c = 0$ and $\delta_c = -\frac{1}{2}$. For the other two positions of the discontinuity that we consider we find $\overline{u}(x_c) = \frac{9}{16} = 0.563$ ($\delta_c = -\frac{1}{4}$) and $\overline{u}(x_c) = \frac{35}{64} = 0.547$ ($\delta_c = -\frac{3}{8}$), cf. the results shown in the Figures 4 and 5.

One could of course define a piecewise linear approximation $\overline{u}$ of $u$ such that $\overline{u}(x_c) = \frac{1}{2}$ for any value of $\alpha$ and $\delta_c$. Obviously, this would require a discretization involving the exact position of the discontinuity, which is not practical. Another possibility is an approximation that is exact at grid points, using $u_j = u(x_j), \forall j$. This leads to an ambiguity if the discontinuity is at a grid point, and to a discontinuous change in the numerical solution if the discontinuity moves across a grid point. These alternative numerical solutions are also not very symmetric.

An interesting property of discretization (6) with grid point solution (7) is that the difference between numerical solution $\overline{u}(x)$ and exact solution $u(x)$ integrated left and right of the discontinuity is equal. This is obviously the result of applying a finite volume approach in combination with the exact definition (5) of discrete function $\overline{u}(x)$

and exact expression (2) of given function $f(x)$:

$$\int_{-\infty}^{x_c} (\overline{u} - u)\, dx = \int_{x_c}^{\infty} (u - \overline{u})\, dx = \frac{\Delta x}{4} \left( \frac{1+\beta}{1-\beta} + \frac{1-\beta}{1+\beta}\, \delta_c^2 \big( 2\delta_c(\beta-1) + \beta - 3 \big) \right) . \quad (15)$$

As expected, the difference between numerical solution

Closest possible approximation is not necessarily the best approximation.

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