

Flux-Limiters, Discontinuous Galerkin Schemes

Ammar H. Hakim (ammар@princeton.edu)¹

¹Princeton Plasma Physics Laboratory, Princeton, NJ

Princeton University, Course AST560, Spring 2021



Nonlinear flux limiters: Getting around Godunov's Theorem

To get around Godunov's Theorem we need to construct a *nonlinear scheme*, even for linear equations. One approach is to use nonlinear flux-limiters:

$$\mathbf{F}_{j+1/2} = \phi(r_{j+1})\mathbf{F}_{j+1/2}^H + (1 - \phi(r_{j+1}))\mathbf{F}_{j+1/2}^L$$

where $\phi(r) > 0$ is a *limiter* function: chooses between *high-order* and *low-order* flux.

- What are the low- and high-order fluxes? For high-order fluxes: use either symmetric or higher-order upwind-biased recovery to construct the flux. For low-order use first-order upwind fluxes.

The first-order upwind flux is “Total-Variation Diminishing” (TVD), $\text{TV}(f^{n+1}) \leq \text{TV}(f^n)$ where “Total-Variation” is defined as:

$$\text{TV}(f) = \sum_j |f_{j+1} - f_j|$$

Nonlinear flux limiters

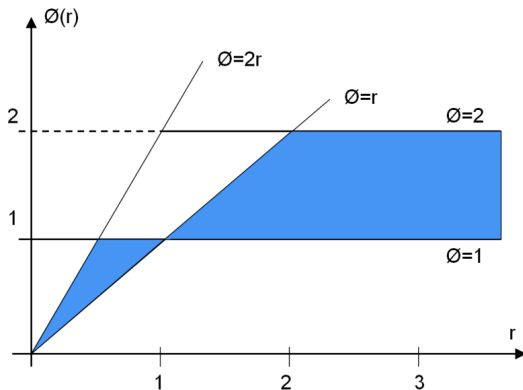
The limiter function $\phi(r)$ depends on an estimate of the *relative slopes* at an interface. For example, one choice is

$$r_{j+1/2} = \frac{\text{slope at upwind-edge}}{\text{slope at } j + 1/2}$$

(For systems of equations one needs limit each eigenvector instead). With this, choose a function that maintains TVD property. Eg, min-mod limiter

$$\phi(r) = \max(0, \min(2r, (1+r)/2, 2)).$$

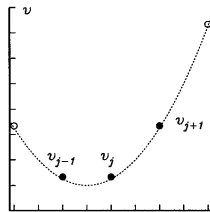
See Wikipedia page https://en.wikipedia.org/wiki/Flux_limiter. (Not very high-quality but gives you a general idea).



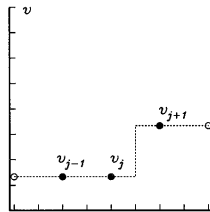
Admissible limiter region for second-order TVD schemes
(Sweby, 1984)

Nonlinear flux limiters: No “Perfect” Limiter!

- Unfortunately, there is no perfect limiter (though some come close to perfection): depends on problem and best to implement many!
- Most limiters “chop off” genuine maxima/minima: notice that $\phi(r < 0) = 0$ which means that if there is a genuine maxima/minima then low-order flux is selected.
- Tricky to distinguish step-function from parabola! “Best” limiter (IMO): Suresh and Huynh, JCP **136**, 83-99 (1997). Not an easy paper to understand.



(a)



(b)

Generalizing recovery: path to discontinuous Galerkin schemes

- In FV scheme we used *cell-averages* to recover interface values for use in numerical fluxes
- What if we store more than just cell-averages? One can imagine in addition, mean-slope, mean-quadratic moments. Lead naturally to the concept of discontinuous Galerkin schemes.

The key connection is the concept of *weak-equality*. Consider an interval I and select a finite-dimensional function space on it, spanned by set of basis functions $\{\psi_k\}$, $k = 1, \dots, N$. Choose an inner product, for example

$$(f, g) \equiv \int_I f(x)g(x) dx.$$

Weak-equality

Definition (Weak equality)

Two functions, f and g are said to be *weakly equal* if

$$(\psi_k, f - g) = 0$$

for all $k = 1, \dots, N$. We denote weak equality by

$$f \doteq g.$$

- When we recovered polynomials across an interface in FV scheme we effectively choose a function space, $\{1\}$, with only *one* basis function!
- In DG we can choose as many as we like: allows significant flexibility in designing accurate and compact schemes; suprisingly accurate for some problems.

What are discontinuous Galerkin schemes?

Discontinuous Galerkin schemes are a class of *Galerkin* schemes in which the solution is represented using *piecewise discontinuous* functions.

- *Galerkin* minimization
- Piecewise *discontinuous* representation

Goal of this lecture is to understand conceptual meaning of discontinuous Galerkin schemes and understand how to use them to solve PDEs. Much is left out as the literature on DG is vast, but will aim to cover key conceptual ideas. Outline

- Discontinuous Galerkin representation, recovery and weak-equalities
- DG scheme for linear advection and extension to Maxwell equations. Aspects of DG for nonlinear problems
- Application of DG to plasma kinetic equations

DG represent state-of-art for solution of PDEs

DG algorithms hot topic in CFD and applied mathematics.

- First introduced by Reed and Hill in 1973 as a conference paper to solve steady-state neutron transport equations. More than 2100 citations.
- Some earlier work on solving *elliptic* equations by Nitsche in 1971 (original paper in German). Introduced the idea of “interior penalty”. Usually, though, DG is not used for elliptic problems. Paradoxically, perhaps DG may be even better for certain elliptic/parabolic problems.
- Key paper for nonlinear systems in multiple dimensions is by Cockburn and Shu (JCP, **141**, 199-224, 1998). More than 1700 citations.
- Almost continuous stream of papers in DG, both for fundamental formulations and applications to physics and engineering problems. This continues to be an active area of research, and at present *DG is under-utilized in plasma physics*.

Essential idea of Galerkin methods: L_2 minimization of errors

There two key ingredients in a Galerkin scheme: selection of a finite-dimensional space of functions and a definition of errors.

- Consider a interval $[-1, 1]$. On this, we can choose Legendre polynomials $P_l(x)$ up to some order $l < N$ as a *basis-set*.
- We need to *define* a way to measure errors on this function space. One way to do this is to select an inner product and then use it to define a norm. For example consider the inner-product

$$(f, g) = \int_{-1}^1 f(x)g(x) dx$$

using which we can define the L_2 norm

$$\|f\|_2 = (f, f)$$

Once we have selected the finite-dimensional space of functions and a norm, we can use it to construct a Galerkin method.

Essential idea of Galerkin methods: L_2 minimization of errors

Consider a general time-dependent problem on $x \in [-1, 1]$:

$$f'(x, t) = G[f]$$

where $G[f]$ is some operator. To approximate it expand $f(x)$ with our basis functions $P_k(x)$,

$$f(x, t) \approx f_h(x, t) = \sum_{k=1}^N f_k(t) P_k(x)$$

This gives discrete system

$$\sum_{k=1}^N f'_k P_k(x) = G[f_h]$$

Question

How to determine f'_k in an optimum manner?

Essential idea of Galerkin methods: L_2 minimization of errors

Answer: Do an L_2 minimization of the error, i.e. find f'_k such that the error as *defined by our selected norm* is minimized.

$$E_N = \left\| \sum_{k=1}^N f'_k P_k(x) - G[f_h] \right\|_2 = \int_{-1}^1 \left[\sum_{k=1}^N f'_k P_k(x) - G[f_h] \right]^2 dx$$

For minimum error $\partial E_N / \partial f'_m = 0$ for all $k = 1, \dots, N$. This leads to the linear system that determines the coefficients f'_k

$$\int_{-1}^1 P_m(x) \left(\sum_{k=1}^N f'_k P_k(x) - G[f_h] \right) dx = 0$$

for all $m = 1, \dots, N$. This will give

$$f'_k = \frac{2k+1}{2} \int_{-1}^1 P_k(x) G[f_h] dx$$

Typical L_2 fit look like for Galerkin scheme?

Consider finding the best-fit on finite-dimensional space for the function $f(x) = 3 + (x - 0.5)^4 + 2x^3 - 5x^2$ on $x \in [-1, 1]$. Choose *normalized* Legendre polynomials as basis functions.

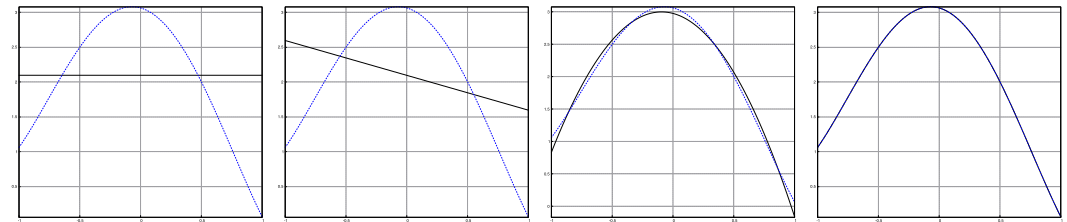
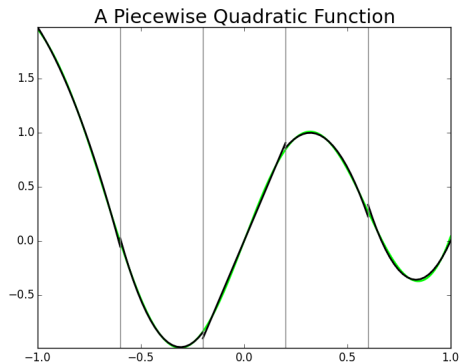
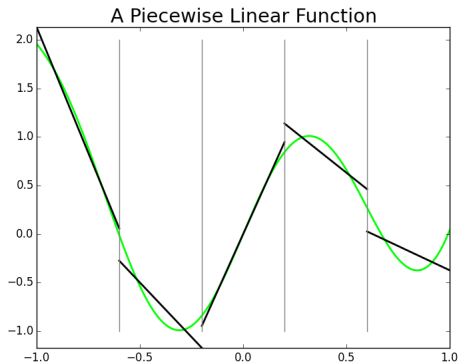


Figure: Best L_2 fit with $p = 0$, $p = 1$, $p = 2$ and $p = 4$ for $f(x) = 3 + (x - 0.5)^4 + 2x^3 - 5x^2$ on $x \in [-1, 1]$.

Typical L_2 fit look like: *discontinuous* Galerkin scheme

In discontinuous Galerkin schemes we split interval into cells and use Galerkin scheme in each cell. This will naturally lead to *discontinuities* across cell boundaries.



Weak-equality and recovery

- It is important to remember that the discontinuous Galerkin solution is a *representation* of the solution and not the solution itself.
- Notice that even a continuous function will, in general, have a discontinuous *representation* in DG.

We can formalize this idea using the concept of *weak-equality*.

Definition (Weak equality)

Two functions, f and g are said to be *weakly equal* if

$$(\psi_k, f - g) = 0$$

for all $k = 1, \dots, N$. We denote weak equality by

$$f \doteq g.$$

Weak-equality and recovery

- Notice that weak-equality depends on the function space as well as the inner-product we selected.
- The Galerkin L_2 minimization is equivalent to, for example, restating that

$$f'(x, t) \doteq G[f]$$

This implies

$$(\psi_k, f'(x, t) - G[f]) = 0$$

which is exactly what we obtained by minimizing the error defined using the L_2 norm.

- Hence, we can say that the *DG scheme only determines the solution in the weak-sense*, that is, all functions that are weakly equal to DG representation can be potentially interpreted as the actual solution.
- This allows a powerful way to construct schemes with desirable properties by *recovering* weakly-equal functions using the DG representations.

Example of recovery: Exponential recovery in a cell

- Consider we have a linear representation of the particle distribution function $f_h(x) = f_0 + xf_1$ in a cell.
- We can use this to *reconstruct* an exponential function that has the desirable property that it is *positive* everywhere in the cell. That is, we want to find

$$\exp(g_0 + g_1x) \doteq f_0 + xf_1$$

- This will lead to a coupled set of nonlinear equations to determine g_0 and g_1
- Note that this process is not always possible: we need $f_0 > 0$ as well as the condition $|f_1| \leq 3f_0$. Otherwise, the f_h is not realizable (i.e. there is no positive distribution function with the same moments as f_h).

Example of recovery: Exponential recovery in a cell

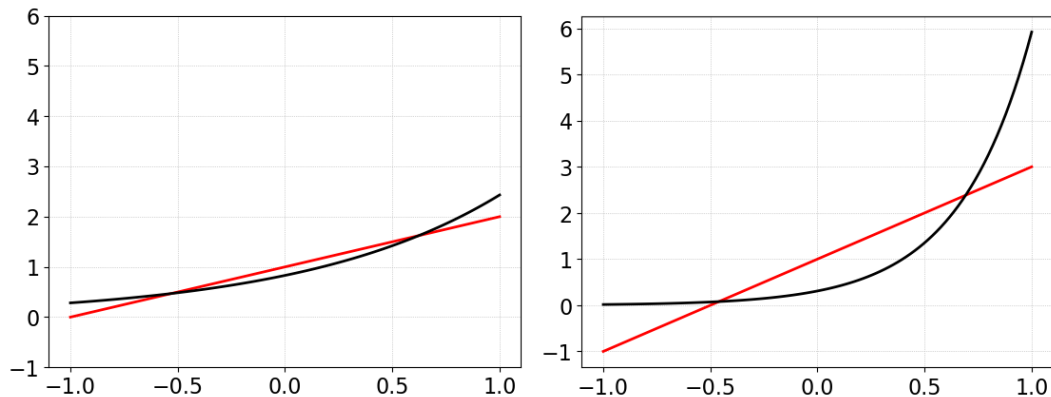


Figure: Recovery of exponential function (black) from linear function (red). Left plot is for $f_0 = 1$, $f_1 = 1$ and right for $f_0 = 1$ and $f_1 = 2$.

Discontinuous Galerkin scheme for linear advection

Consider the 1D passive advection equation on $I \in [L, R]$

$$\frac{\partial f}{\partial t} + \lambda \frac{\partial f}{\partial x} = 0$$

with λ the constant advection speed. $f(x, t) = f_0(x - \lambda t)$ is the exact solution, where $f_0(x)$ is the initial condition. Designing a good scheme is much harder than it looks.

- Discretize the domain into elements $I_j \in [x_{j-1/2}, x_{j+1/2}]$
- Pick a finite-dimensional function space to represent the solution. For DG we usually pick polynomials in each cell but allow discontinuities across cell boundaries
- Expand $f(x, t) \approx f_h(x, t) = \sum_k f_k(t) w_k(x)$.

Find the coefficients that minimize the L_2 norm of the residual

The discrete problem in DG is stated as: find f_h in the function space such that for each basis function φ we have

$$\int_{I_j} \varphi \left(\frac{\partial f_h}{\partial t} + \lambda \frac{\partial f_h}{\partial x} \right) dx = 0.$$

Integrating by parts leads to the discrete *weak-form*

$$\int_{I_j} \varphi \frac{\partial f_h}{\partial t} dx + \lambda \varphi_{j+1/2} \hat{F}_{j+1/2} - \lambda \varphi_{j-1/2} \hat{F}_{j-1/2} - \int_{I_j} \frac{d\varphi}{dx} \lambda f_h dx = 0.$$

Here $\hat{F} = \hat{F}(f_h^+, f_h^-)$ is the consistent *numerical flux* on the cell boundary. Integrals are performed using high-order quadrature schemes.

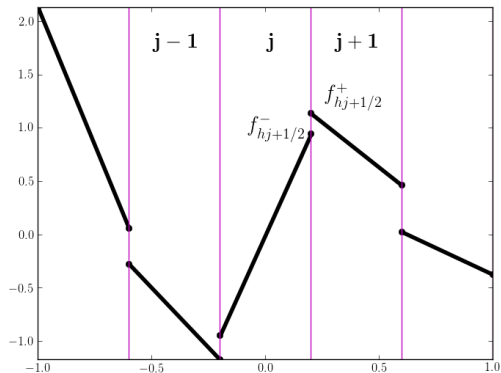
Need to select numerical flux

- Take averages (central fluxes)

$$\hat{F}(f_h^+, f_h^-) = \frac{1}{2}(f_h^+ + f_h^-)$$

- Use upwinding (upwind fluxes)

$$\begin{aligned}\hat{F}(f_h^+, f_h^-) &= f_h^- & \lambda > 0 \\ &= f_h^+ & \lambda < 0\end{aligned}$$



Example: Piecewise constant basis functions

- A central flux with piecewise constant basis functions leads to the familiar central difference scheme

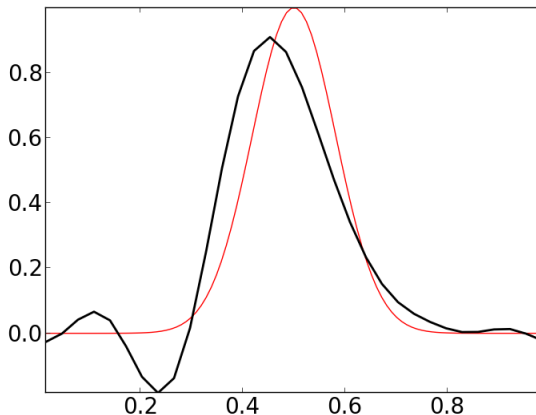
$$\frac{\partial f_j}{\partial t} + \lambda \frac{f_{j+1} - f_{j-1}}{2\Delta x} = 0$$

- An upwind flux with piecewise constant basis functions leads to the familiar upwind difference scheme (for $\lambda > 0$)

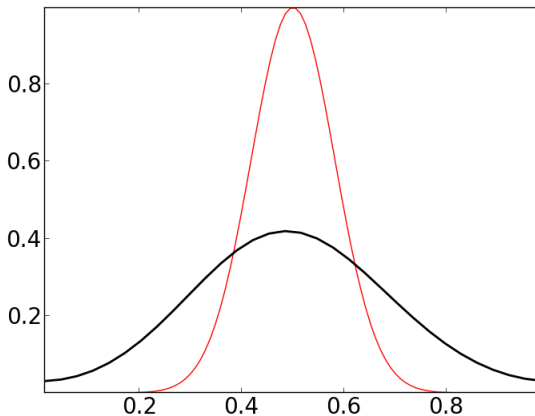
$$\frac{\partial f_j}{\partial t} + \lambda \frac{f_j - f_{j-1}}{\Delta x} = 0$$

Solution is advanced in time using a suitable ODE solver, usually strong-stability preserving Runge-Kutta methods. (See G2 website)

Example: Piecewise constant basis functions with central flux



Example: Piecewise constant basis functions with upwind flux



Passive advection with piecewise linear basis functions

To get better results, we can use piecewise linear polynomials instead. That is, select the basis functions

$$\varphi \in \{1, 2(x - x_j)/\Delta x\}$$

In terms of which the solution in each cell is expanded as $f_j(x, t) = f_{j,0} + 2f_{j,1}(x - x_j)/\Delta x$. With this, some algebra shows that we have the update formulas for *each stage* of a Runge-Kutta method

$$\begin{aligned}f_{j,0}^{n+1} &= f_{j,0}^n - \sigma \left(\hat{F}_{j+1/2} - \hat{F}_{j-1/2} \right) \\f_{j,1}^{n+1} &= f_{j,1}^n - 3\sigma \left(\hat{F}_{j+1/2} + \hat{F}_{j-1/2} \right) + 6\sigma f_{j,0}\end{aligned}$$

where $\sigma \equiv \lambda \Delta t / \Delta x$. As these are explicit schemes we need to ensure time-step is sufficiently small. Usually, we need to ensure $\sigma = \lambda \Delta t / \Delta x \leq 1/(2p + 1)$.

Passive advection with piecewise linear basis functions

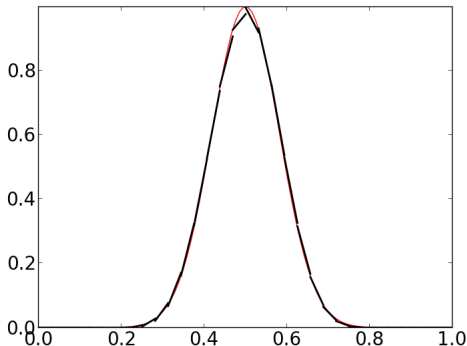


Figure: Advection equation solution (black) compared to exact solution (red) with upwind fluxes and piecewise linear basis functions.

Properties of the discrete equations

From the continuous passive advection equation we can show that, on a periodic domain the total particles are conserved

$$\frac{d}{dt} \int_I f \, dx = 0$$

Also, the L_2 norm of the solution is also conserved

$$\frac{d}{dt} \int_I \frac{1}{2} f^2 \, dx = 0$$

We would like to know if our discrete scheme *inherits or mimics these properties*. Sometimes, methods in which the discrete scheme inherit important properties from the continuous equations are called *mimetic* methods. However, note that in general it is impossible to inherit *all* properties and often it is not desirable to do so.

To prove properties start from discrete weak-form

To understand properties of the scheme we must (obviously) use the *discrete weak-form* as the starting point.

$$\int_{I_j} \varphi \frac{\partial f_h}{\partial t} dx + \lambda \varphi_{j+1/2} \hat{F}_{j+1/2} - \lambda \varphi_{j-1/2} \hat{F}_{j-1/2} - \int_{I_j} \frac{d\varphi}{dx} \lambda f_h dx = 0.$$

A general technique is to use a function belonging to the *finite-dimensional function space* as the test function φ in the discrete weak-form.

Example: consider we set $\varphi = 1$. Then we get

$$\sum_j \int_{I_j} \frac{\partial f_h}{\partial t} dx + \lambda \sum_j \left(\hat{F}_{j+1/2} - \hat{F}_{j-1/2} \right) = 0.$$

The second term sums to zero and so we have shown that

$$\frac{d}{dt} \sum_j \int_{I_j} f_h dx = 0.$$

To prove properties start from discrete weak-form

Now, consider we use the *solution itself* as the test function. We can do this as the solution, by definition, belongs to the finite-dimensional function space. We get

$$\sum_j \int_{I_j} f_h \frac{\partial f_h}{\partial t} dx + \sum_j \left(f_{hj+1/2}^- \hat{F}_{j+1/2} - f_{hj-1/2}^+ \hat{F}_{j-1/2} \right) - \sum_j \int_{I_j} \frac{df_h}{dx} f_h dx = 0$$

We can write the last term as

$$\sum_j \int_{I_j} \frac{1}{2} \frac{d}{dx} f_h^2 dx = \frac{1}{2} \sum_j \left[\left(f_{hj+1/2}^- \right)^2 - \left(f_{hj-1/2}^+ \right)^2 \right]$$

If we use *upwind fluxes* we can show that we get

$$\frac{d}{dt} \sum_j \int_{I_j} f_h^2 dx = - \sum_j \left(f_{hj+1/2}^- - f_{hj-1/2}^+ \right)^2 \leq 0.$$

Hence, the L_2 norm of the solution *will decay and not remain constant*. However, this is the desirable behavior as it ensures L_2 stability of the discrete system. With central fluxes the L_2 norm is conserved. (Prove this)

Summary of DG schemes for passive advection equation

- Pick basis functions. These are usually piecewise polynomials, but could be other suitable functions.
- Construct discrete weak-form using integration by parts.
- Pick suitable numerical fluxes for the surface integrals.
- Use Runge-Kutta (or other suitable) schemes for evolving the equations in time.
- To prove properties of the scheme, start from the discrete weak-form and use appropriate test-functions and simplify.

How to discretize parabolic equations with DG?

- DG is traditionally used to solve hyperbolic PDEs. However, DG is also very good for the solution of parabolic PDEs.
- One challenge here is that parabolic PDEs have *second* derivatives and it is not clear at first how a discontinuous representation can allow solving such systems.

Consider the diffusion equation (subscripts represent derivatives)

$$f_t = f_{xx}$$

Choose function space and multiply by test function in this space to get weak form

$$\int_{I_j} \varphi f_t dx = \varphi f_x \Big|_{x_{j-1/2}}^{x_{j+1/2}} - \int_{I_j} \varphi_x f_x dx.$$

In DG, as f is discontinuous, it is not clear how to compute the derivative across the discontinuity at the cell interface in the first term. (See SimJ JE16).

Lets revisit weak-equality and recovery

Definition (Weak equality)

Two functions, f and g are said to be *weakly equal* if

$$(\psi_k, f - g) = 0$$

for all $k = 1, \dots, N$. We denote weak equality by

$$f \doteq g.$$

Recall that the DG solution is only a *representation* of the solution and not the solution itself. Hence, we can consider the following “inverse” problem: given a discontinuous solution across two cells, is it possible to *recover* a *continuous representation* that can then be used in the above weak-form?

Use weak-equality to *recover* continuous function

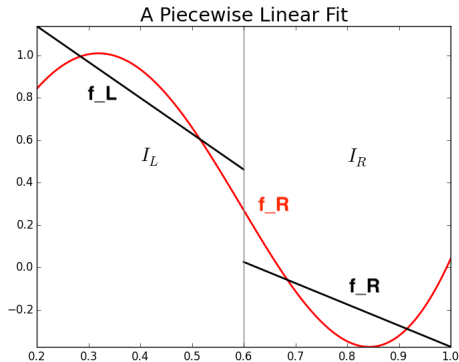


Figure: Given piecewise linear representation (black) we want to recover the continuous function (red) such that **moments of recovered and linear representation are the same in the respective cells.**

Use weak-equality to *recover* continuous function

- Consider recovering \hat{f} on the interval $I = [-1, 1]$, from a function, f , which has a single discontinuity at $x = 0$.
- Choose some function spaces \mathcal{P}_L and \mathcal{P}_R on the interval $I_L = [-1, 0]$ and $I_R = [0, 1]$ respectively.
- Reconstruct a continuous function \hat{f} such that

$$\begin{aligned}\hat{f} &\doteq f_L \quad x \in I_L \quad \text{on } \mathcal{P}_L \\ \hat{f} &\doteq f_R \quad x \in I_R \quad \text{on } \mathcal{P}_R.\end{aligned}$$

where $f = f_L$ for $x \in I_L$ and $f = f_R$ for $x \in I_R$.

- To determine \hat{f} , use the fact that given $2N$ pieces of information, where N is the number of basis functions in $\mathcal{P}_{L,R}$, we can construct a polynomial of maximum order $2N - 1$. We can hence write

$$\hat{f}(x) = \sum_{m=0}^{2N-1} \hat{f}_m x^m.$$

Plugging this into the weak-equality relations gives a *linear* system for \hat{f}_m .

Use recovered function in weak-form

Once we have determined \hat{f} we can use this in the discrete weak-form of the diffusion equation:

$$\int_{I_j} \varphi f_t dx = \varphi \hat{f}_x \Big|_{x_{j-1/2}}^{x_{j+1/2}} - \int_{I_j} \varphi_x f_x dx.$$

Note that now as \hat{f} is continuous at the cell interface there is no issue in computing its derivative. We can, in fact, do a second integration by parts to get another discrete weak-form

$$\int_{I_j} \varphi f_t dx = (\varphi \hat{f}_x - \varphi_x \hat{f}) \Big|_{x_{j-1/2}}^{x_{j+1/2}} + \int_{I_j} \varphi_{xx} f dx.$$

This weak-form has certain advantages as the second term does not contain derivatives (which may be discontinuous at cell boundary).