Modified equations and $\frac{\pi^2}{6}$

Mats Vermeeren

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berlin

Berlin
Mathematical
School

Basel Problem

In 1644, Pietro Mengoli wondered

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = ?$$

Solved by Leonhard Euler in 1735: $\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}$.

Basel Problem

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Today many proofs are known.

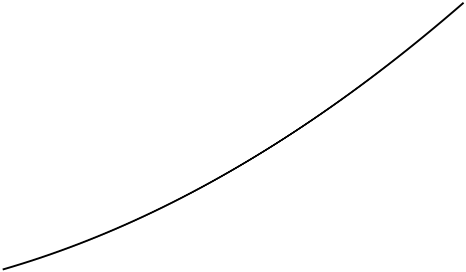
One proof relies on the series expansion

$$\left(\arcsin \frac{h}{2}\right)^2 = \frac{1}{2} \sum_{k=1}^{\infty} \frac{(k-1)!^2}{(2k)!} h^{2k}.$$

Setting $h = 1$ in this expansion + some algebraic manipulations, yields the desired result.

→ Relocates the difficulty: proving this expansion is not easy.

So let's talk about something else



- Given is (a solution of) a differential equation.

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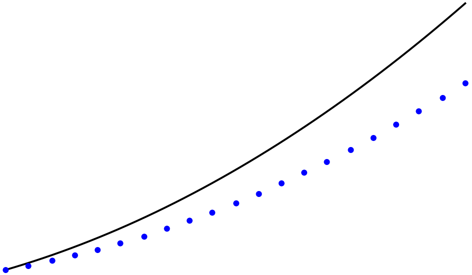

- Given is (a solution of) a differential equation.
- And a numerical approximation thereof.

  We make an error, but how to compare discrete with continuous?

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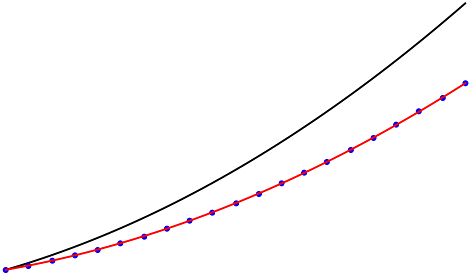


- Given is (a solution of) a differential equation.
- And a numerical approximation thereof.

  We make an error, but how to compare discrete with continuous?
- Can we find a modification of the differential equation, that (has a solution that) interpolates the discrete system?

Modified equation for a very simple system

Consider the ODE

$$\dot{x}(t) = -x(t)$$

and its explicit Euler discretization with step size h

$$\frac{x_{j+1} - x_j}{h} = -x_j.$$

Modified equation

$$\dot{x} = F(x; h)$$

whose solutions satisfy the difference equation, in the sense that

$$x(t+h) - x(t) = -hx(t)$$

The right hand side is a power series,

$$F(x; h) = f_0(x) + hf_1(x) + h^2 f_2(x) + \ldots .$$

Modified equation for a very simple system

$$x(t+h) - x(t) = -hx(t)$$
$$\Rightarrow \quad h\dot{x}(t) + \frac{h^2}{2}\ddot{x}(t) + \frac{h^3}{6}x^{(3)}(t) + \ldots = -hx(t).$$

The higher derivatives can be written as

$$\begin{aligned}
\ddot{x} &= F'(x;h)F(x;h) \\
&= \left(f_0'(x) + hf_1'(x) + h^2 f_2'(x) + \ldots\right)\left(f_0(x) + hf_1(x) + h^2 f_2(x) + \ldots\right), \\
x^{(3)} &= F''(x;h)F(x;h)^2 + F'(x;h)^2 F(x;h) \\
&= \left(f_0''(x) + hf_1''(x) + h^2 f_2''(x) + \ldots\right)\left(f_0(x) + hf_1(x) + h^2 f_2(x) + \ldots\right)^2 \\
&\quad + \left(f_0'(x) + hf_1'(x) + h^2 f_2'(x) + \ldots\right)^2\left(f_0(x) + hf_1(x) + h^2 f_2(x) + \ldots\right)
\end{aligned}$$

$$\begin{aligned}
\Rightarrow h\left(f_0 + hf_1 + h^2 f_2 + \ldots\right) + \frac{h^2}{2}\left(f_0' f_0 + hf_1' f_0 + hf_0' f_1 + \ldots\right) \\
+ \frac{h^3}{6}\left(f_0'' f_0^2 + f_0'^2 f_0 + \ldots\right) + \ldots = -hx,
\end{aligned}$$

Modified equation for a very simple system

Grouping terms by order in h we find

$$h(f_0 + x) + h^2\left(f_1 + \frac{1}{2}f_0'f_0\right) + h^3\left(f_2 + \frac{1}{2}f_1'f_0 + \frac{1}{2}f_0'f_1 + \frac{1}{6}f_0''f_0^2 + \frac{1}{6}f_0'^2 f_0\right) + \ldots = 0.$$

For a power series to be equal to zero, all of the coefficients must be zero. We find

$$f_0(x) = -x, \qquad f_1(x) = -\frac{1}{2}x, \qquad f_2(x) = -\frac{1}{3}x, \qquad \ldots$$

hence the modified equation is

$$\dot{x} = -x - \frac{h}{2}x - \frac{h^2}{3}x - \ldots.$$

- Leading order term agrees with the original differential equation.
- Higher order terms reflect the discretization error.

What have we gained through all this work?

- $x_{j+1} = x_j - hx_j$ is linear, so it can be solved exactly
- Here the modified equation doesn't provide any new information.

What have we gained through all this work?

- $x_{j+1} = x_j - hx_j$ is linear, so it can be solved exactly
- Here the modified equation doesn't provide any new information.
- However, the same procedure can be applied to nonlinear difference equations too.

  (Terms tend to become more and more complicated as the order in h increases.)

Definition

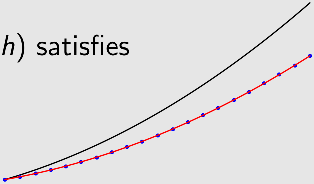
The differential equation $\dot{x} = F(x;h)$ is a modified equation for the difference equation

$$\Psi(x_j, x_{j+1}; h) = 0$$

if (for small $h > 0$) every solution x of $\dot{x} = F(x;h)$ satisfies

$$\Psi\big(x(t), x(t+h); h\big) = 0$$

for all $t \in \mathbb{R}$.



Second order ODEs

Definition

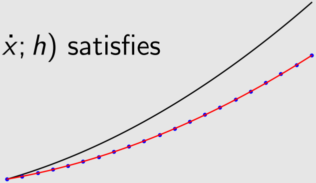
The differential equation $\ddot{x} = F(x, \dot{x}; h)$ is a modified equation for the second order difference equation

$$\Psi(x_{j-1}, x_j, x_{j+1}; h) = 0$$

if (for small $h > 0$) every solution x of $\ddot{x} = F(x, \dot{x}; h)$ satisfies

$$\Psi\big(x(t-h), x(t), x(t+h); h\big) = 0$$

for all $t \in \mathbb{R}$.



In general F is a formal power series in h. To avoid convergence issues one can truncate at an arbitrary order k and relax the condition to

$$\Psi\big(x(t-h), x(t), x(t+h); h\big) = \mathcal{O}(h^k)$$

Harmonic oscillator

Consider the ODE

$$\ddot{x} = -x$$

and its Störmer-Verlet discretization

$$\frac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = -x_j.$$

The modified equation here is unusually simple, not $\ddot{x} = F(x, \dot{x}; h)$ but

$$\ddot{x} = F_h(x) = f_0(x) + h^2 f_2(x) + h^4 f_4(x) + \cdots .$$

The higher derivatives then look like

$$\begin{aligned}
x^{(3)} &= F_h' \dot{x}, \\
x^{(4)} &= F_h'' \dot{x}^2 + F_h' F_h, \\
x^{(5)} &= F_h^{(3)} \dot{x}^3 + 3F_h'' F_h \dot{x} + F_h'^2 \dot{x}, \\
x^{(6)} &= F_h^{(4)} \dot{x}^4 + 6F_h^{(3)} F_h \dot{x}^2 + 5F_h'' F_h' \dot{x}^2 + 3F_h'' F_h^2 + F_h'^2 F_h,
\end{aligned}$$

Harmonic oscillator

Using Taylor expansion we find

$$x(t \pm h) = x \pm h\dot{x} + \frac{h^2}{2}\ddot{x} \pm \frac{h^3}{6}x^{(3)} + \frac{h^4}{24}x^{(4)} \pm \frac{h^5}{120}x^{(5)} + \frac{h^6}{720}x^{(6)} + \cdots .$$

Plug this into the difference equation

$$-hx(t) = x(t+h) - 2x(t) + x(t-h).$$

and expand:

$$\begin{aligned}
-h^2 x &= h^2 \ddot{x} + \frac{h^4}{12}x^{(4)} + \frac{h^6}{360}x^{(6)} + \ldots \\
&= h^2(f_0 + h^2 f_2 + h^4 f_4) + \frac{h^4}{12}\left(f_0'' \dot{x}^2 + h^2 f_2'' \dot{x}^2 + f_0' f_0 + h^2 f_0' f_2 + h^2 f_2' f_0 \right) \\
&\qquad + \frac{h^6}{360}\left(f_0^{(4)} \dot{x}^4 + 6 f_0^{(3)} f_0 \dot{x}^2 + 5 f_0'' f_0' \dot{x}^2 + 3 f_0'' f_0^2 + f_0'^2 f_0 \right) + \ldots \\
&= h^2 f_0 + h^4 \left(f_2 + \frac{1}{12}\left(f_0'' \dot{x}^2 + f_0' f_0 \right) \right) \\
&\qquad + h^6 \left(f_4 + \frac{1}{\ldots}\left(f_2'' \dot{x}^2 + f_0' f_2 + f_2' f_0 \right) + \frac{1}{\ldots}\left(f_0^{(4)} \dot{x}^4 + 6 f_0^{(3)} f_0 \dot{x}^2 + 5 \right.\right.
\end{aligned}$$

Harmonic oscillator

Matching terms of the same order in h, we can solve recursively for the f_i:

$$f_0(x) = -x, \qquad f_2(x) = -\frac{x}{12}, \qquad f_4(x) = -\frac{x}{90}, \qquad \cdots .$$

Hence the modified equation is

$$\ddot{x} = -x - \frac{h^2}{12}x - \frac{h^4}{90}x - \ldots .$$

In other examples, calculations quickly become complicated, but the same construction works in general. This shows that:

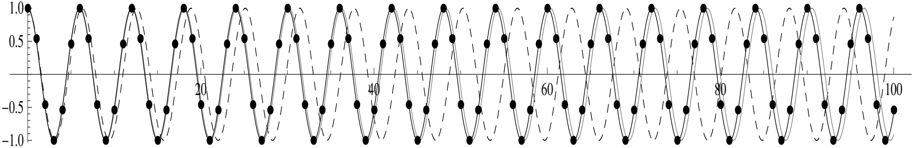
Theorem

If there exists a modified equation that can be represented as a power series

$$\ddot{x} = f_0(x,\dot{x}) + hf_1(x,\dot{x}) + h^2 f_2(x,\dot{x}) + h^3 f_3(x,\dot{x}) + \ldots$$

then it is unique.

Numerical experiment for the harmonic oscillator



• • • • solution of $x_{j+1} - 2x_j + x_{j-1} = -h^2 x_j$

- - - - - - solution of $\ddot{x} = -x$ (original ODE)

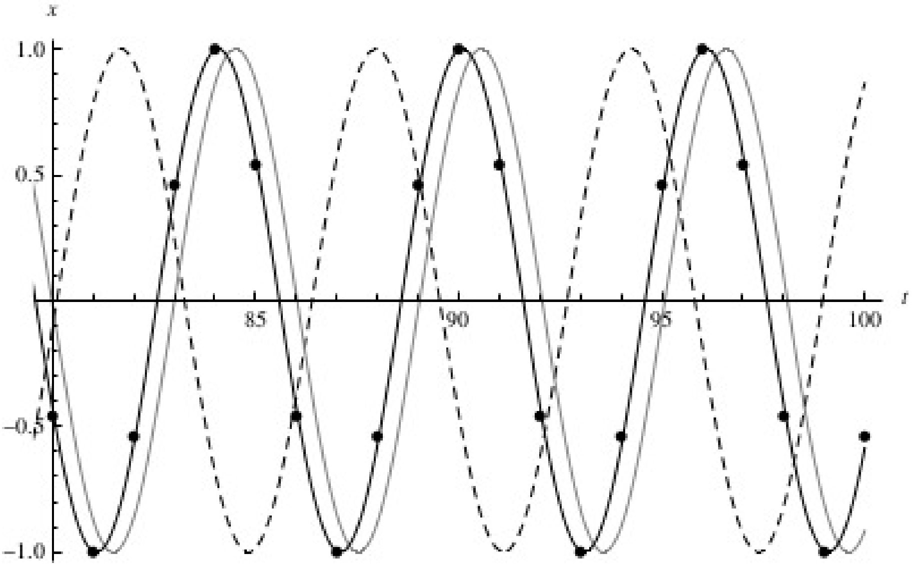
——— (grey) solution of $\ddot{x} = -x - \frac{h^2}{12}x$

——— (black) solution of $\ddot{x} = -x - \frac{h^2}{12}x - \frac{h^4}{90}x$

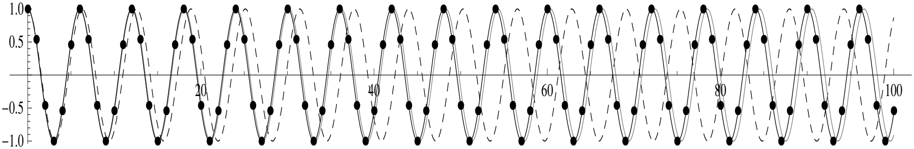
(truncations of mod eqn)

all with $h = 1$.

Tail end of the graph



Discrete system with $h = 1$ has period 6



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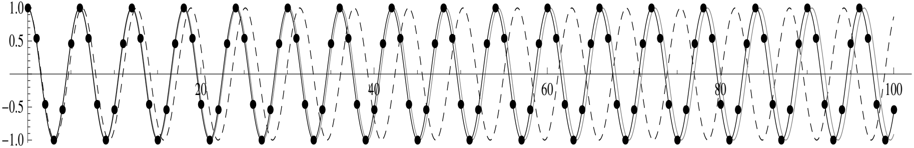

The modified equation is $\ddot{x} = -\frac{\pi^2}{9}x$.

Proof. Because the difference equation is linear, we can solve it exactly:

$$x_j = Ae^{-2ij\theta} + Be^{2ij\theta},$$

where $\theta = \arcsin\left(\frac{h}{2}\right)$. The interpolating curve

$$x(t) = Ae^{-2it\theta/h} + Be^{2it\theta/h}$$

satisfies the differential equation

$$\ddot{x} = -\left(\frac{2}{h}\arcsin\left(\frac{h}{2}\right)\right)^2 x. \qquad \square$$

Back to Basel

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = ?$$

We want to show

$$\left(\arcsin \frac{h}{2} \right)^2 = \frac{1}{2} \sum_{k=1}^{\infty} \frac{(k-1)!^2}{(2k)!} h^{2k} \qquad (*)$$

The modified equation in our example can be written as

- a closed-form expression involving the LHS of $(*)$,
- a power series, where the coefficients can be calculated recursively.

Still needed:

- explicit expressions for the coefficients of that power series, to identify it with the RHS of $(*)$.

Determining the coefficients of the power series

For any smooth curve x, a second difference can be expanded as

$$\begin{aligned} &x(t-jh) - 2x(t) + x(t+jh) \\ &= (jh)^2 \ddot{x}(t) + \frac{2(jh)^4}{4!} x^{(4)}(t) + \ldots + \frac{2(jh)^{2k}}{(2k)!} x^{(2k)}(t) + \mathcal{O}(h^{2k+2}), \end{aligned}$$

or, in matrix form,

$$\begin{pmatrix} x(t-h) - 2x(t) + x(t+h) \\ x(t-2h) - 2x(t) + x(t+2h) \\ \vdots \\ x(t-kh) - 2x(t) + x(t+kh) \end{pmatrix} = \begin{pmatrix} 1 & 1 & \ldots & 1 \\ 2^2 & 2^4 & \ldots & 2^{2k} \\ \vdots & \vdots & \ddots & \vdots \\ k^2 & k^4 & \ldots & k^{2k} \end{pmatrix} \begin{pmatrix} h^2 \ddot{x}(t) \\ \frac{2h^4}{4!} x^{(4)}(t) \\ \vdots \\ \frac{2h^{2k}}{(2k)!} x^{(2k)}(t) \end{pmatrix} + \mathcal{O}(h^{2k+2}).$$

Determining the coefficients of the power series

Using Cramer's rule we solve for $h^2\ddot{x}(t)$,

$$h^2\ddot{x}(t) = \frac{\begin{vmatrix} x(t-h) - 2x(t) + x(t+h) & 1 & \dots & 1 \\ x(t-2h) - 2x(t) + x(t+2h) & 2^4 & \dots & 2^{2k} \\ \vdots & \vdots & \ddots & \vdots \\ x(t-kh) - 2x(t) + x(t+kh) & k^4 & \dots & k^{2k} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \dots & 1 \\ 2^2 & 2^4 & \dots & 2^{2k} \\ \vdots & \vdots & \ddots & \vdots \\ k^2 & k^4 & \dots & k^{2k} \end{vmatrix}} + \mathcal{O}(h^{2k+2}).$$

In the denominator we have a Vandermonde determinant that equals

$$(k!)^2 \prod_{1 \le i < j \le k} (j^2 - i^2).$$

The numerator

$$\begin{vmatrix} x(t-h)-2x(t)+x(t+h) & 1 & \dots & 1 \\ x(t-2h)-2x(t)+x(t+2h) & 2^4 & \dots & 2^{2k} \\ \vdots & \vdots & \ddots & \vdots \\ x(t-kh)-2x(t)+x(t+kh) & k^4 & \dots & k^{2k} \end{vmatrix} = ?$$

Once more we are helped by the linearity of the difference equation: the sum $x_{i-j}+x_{i+j}$ can be written as

$$x_{i-j}+x_{i+j} = 2T_k\left(1-\frac{h^2}{2}\right)x_i,$$

where T_k denotes the k-th Chebyshev polynomial of the first kind.

Hence any solution of the modified equation satisfies

$$\begin{aligned} x(t-jh)+x(t+jh) &= 2T_j\left(1-\frac{h^2}{2}\right)x(t) \\ &= (-1)^k h^{2j} x(t) + \text{terms of lower order in } h. \end{aligned}$$

The numerator

Let the curve x be a solution of the modified equation. Then the h^{2k}-term of

$$\begin{vmatrix} x(t-h)-2x(t)+x(t+h) & 1 & \dots & 1 \\ x(t-2h)-2x(t)+x(t+2h) & 2^4 & \dots & 2^{2k} \\ \vdots & \vdots & \ddots & \vdots \\ x(t-kh)-2x(t)+x(t+kh) & k^4 & \dots & k^{2k} \end{vmatrix}$$

is

$$\begin{vmatrix} 0 & 1 & \dots & 1 \\ 0 & 2^4 & \dots & 2^{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & (k-1)^4 & \dots & (k-1)^{2k} \\ (-1)^k x(t) & k^4 & \dots & k^{2k} \end{vmatrix} = - \begin{vmatrix} 1 & \dots & 1 \\ 2^4 & \dots & 2^{2k} \\ \vdots & \ddots & \vdots \\ (k-1)^4 & \dots & (k-1)^{2k} \end{vmatrix} x(t)$$

The numerator

Let the curve x be a solution of the modified equation. Then the h^{2k}-term of

$$\begin{vmatrix} x(t-h)-2x(t)+x(t+h) & 1 & \dots & 1 \\ x(t-2h)-2x(t)+x(t+2h) & 2^4 & \dots & 2^{2k} \\ \vdots & \vdots & \ddots & \vdots \\ x(t-kh)-2x(t)+x(t+kh) & k^4 & \dots & k^{2k} \end{vmatrix}$$

is

$$\begin{vmatrix} 0 & 1 & \dots & 1 \\ 0 & 2^4 & \dots & 2^{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & (k-1)^4 & \dots & (k-1)^{2k} \\ (-1)^k x(t) & k^4 & \dots & k^{2k} \end{vmatrix} = - \begin{vmatrix} 1 & \dots & 1 \\ 2^4 & \dots & 2^{2k} \\ \vdots & \ddots & \vdots \\ (k-1)^4 & \dots & (k-1)^{2k} \end{vmatrix} x(t)$$

$$= -((k-1)!)^4 \left(\prod_{1 \leq i < j \leq k-1} \left(j^2 - i^2\right) \right) x(t).$$

The coefficients of the power series

Expansion of $x(t-jh) - 2x(t) + x(t+jh)$ $(j = 1, \ldots, k)$ leads to

$$h^2 \ddot{x}(t) = \frac{|*|}{|*|} + \mathcal{O}(h^{2k+2}).$$

For solutions of the modified equation, we found that the h^{2k}-term of $\frac{|*|}{|*|}$ is

$$-\frac{((k-1)!)^4 \displaystyle\prod_{1 \leq i < j \leq k-1} (j^2 - i^2)}{(k!)^2 \displaystyle\prod_{1 \leq i < j \leq k} (j^2 - i^2)} x(t) = -\frac{2(k-1)!^2}{(2k)!} h^{2k-2} x(t).$$

We have found explicit expressions for the terms of the modified equation!

In its power series form, the modified equation is

$$\ddot{x} = -\sum_{k=1}^{\infty} \frac{2(k-1)!^2}{(2k)!} h^{2k-2} x.$$

Fitting the pieces together

We have two expressions for the modified equation:

$$\ddot{x} = -\sum_{k=1}^{\infty} \frac{2(k-1)!^2}{(2k)!} h^{2k-2} x,$$

$$\ddot{x} = -\left(\frac{2}{h}\arcsin\left(\frac{h}{2}\right)\right)^2 x.$$

Since the modified equation, written in the form "$\ddot{x} =$ power series" is unique, it follows that both expressions coincide,

$$-\left(\frac{2}{h}\arcsin\frac{h}{2}\right)^2 = -\sum_{k=1}^{\infty} \frac{2(k-1)!^2}{(2k)!} h^{2k-2}.$$

This proves:

Theorem

$$\left(\arcsin\frac{h}{2}\right)^2 = \frac{1}{2}\sum_{k=1}^{\infty} \frac{(k-1)!^2}{(2k)!} h^{2k}.$$

Fitting the pieces together

Plugging in $h = 1$ we find

$$\sum_{k=1}^{\infty} \frac{(k-1)!^2}{(2k)!} = \frac{\pi^2}{18}.$$

By elementary (but nontrivial) calculations one can show that

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = 3 \sum_{k=1}^{\infty} \frac{(k-1)!^2}{(2k)!},$$

which leads to the conclusion that

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}.$$

We worked too hard

The closed-form expression of the modified equation

$$\ddot{x} = -\left(\frac{2}{h}\arcsin\left(\frac{h}{2}\right)\right)^2 x$$

is not needed to arrive at $\displaystyle\sum_{k=1}^{\infty}\frac{1}{k^2} = \frac{\pi^2}{6}$.

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If is sufficient to known that

- The modified equation is $\displaystyle\ddot{x} = -\sum_{k=1}^{\infty}\frac{2(k-1)!^2}{(2k)!}h^{2k-2}x.$
- Solutions to the discrete system $x_{j+1} - 2x_j + x_{j-1} = -h^2 x_j$ for $h = 1$ are 6-periodic, and hence solutions to the modified equation as well.

From these two facts it follows that $\displaystyle\sum_{k=1}^{\infty}\frac{(k-1)!^2}{(2k)!} = \frac{\pi^2}{18}$

Summary

Modified equations

- Important tool in numerical analysis.
- Reversing the discretization ("Backward error analysis"):

  we look for a differential equation for which the discretization would have been exact.
- Usually given by formal power series.

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- Usually given by formal power series.

Specific example where the power series converges:

- Properties of the discrete system can be useful to evaluate it.
- Reverses the direction of thinking once more:

  we use the discrete system to learn about the continuous one.
- Same direction as numerical integration, but now everything is exact:

  we use the periodicity to evaluate the power series in the rhs.

Relevance

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I don't know . . .

At first submission (2015)

- Reviewer #2 strikes again:

  "[it is] far from utility, beauty and necessity"

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Many iterations later:

- to appear in the Mathematical Intelligencer
- Pre-print:
  V. Modified equations and the Basel problem. `arXiv:1506.05288v3`

But I still don't know ...