# Explicit approximate Green's function for parabolic equations.

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# Collaborators

- Victor Nistor (PSU Math ),
- Nick Costanzino (PSU Math, Postdoc),
- Wen Cheng (PSU Math, Graduate student),
- John Liechty (PSU Business School), MCMC methods,
- Radu Costantinescu (JPMorgan), financial models.

# Parabolic equations

- Solve the parabolic equation in $\mathbb{R}^N$:

$$\begin{cases} \partial_t u - Lu = g, & t > 0, \\ u(0) = h. \end{cases}$$

where

$$L = \sum_{i,j} a^{ij}(x)\partial_i\partial_j + \sum_j b^j(x)\partial_j + c(x),$$

with smooth, bounded coefficients, and $A = [a^{ij}]$ symmetric and positive definite ($\Rightarrow$ L is strongly elliptic).

- Solution in term of Green's function or fundamental solution:

$$u(x,t) = \int \mathcal{G}_t^L(x,y)\, f(y)\, dy.$$

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$$u(x,t) = \int \mathcal{G}_t^L(x,y)\, f(y)\, dy.$$

- Goal is to obtain approximations of the Green's function, explicitly computable and accurate to any order as $t \to 0^+$.
- Approximation obtained via *elementary* methods, easily implemented algorithmically.
- Method works for time-dependent coefficients (W. Cheng's PhD Thesis), and in certain free-boundary problems.
- Approximate solutions for **semi-linear** equations by fixed-point method (e.g. from non-linear Feynmann-Kac formula).
- Application to parameter estimation. E.g., reconstruct volatility from prices on contingent claims (V. Isakov for Black-Scholes)

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# Applications/Extensions

- When $b^j(x) \neq 0$, $\partial_t - L$ is a **Fokker-Planck** or **Forward Kolmogorov** operator $\Rightarrow$ evolution of the p.d.f associated to the following stochastic process:

$$dX = b(X)\,dt + \sqrt{A(X)}\,dW(X), \quad W \text{ Brownian Motion.}$$

(Statistical Mechanics, Probability, ...).

- Can allow for certain singular coefficients, if bounded in the Varadhan metric $A^{-1}(x)$ and the metric is of bounded geometry (curvature and its derivatives bounded).

Example: $Lu(x) = \sigma(x)\,x^2\partial_x^2 u(x) + 2r(x)(x\partial_x u(x) - u(x))$,

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# Well-posedness

- $\mathcal{G}^L(x,y)$ is the Green's function for $\partial_t - L$, *i.e.*, the distributional kernel of the solution operator $e^{tL}$.
- Use also notation $T(x,y)$ to denote the kernel of operator $T$, if a smooth function.
- Error estimates sought in largest space where uniqueness holds $\Rightarrow$ *exponentially weighted* Sobolev space:

$$W_a^{r,p}(\mathbb{R}^N) := e^{-a\langle x\rangle} W^{r,p}(\mathbb{R}^N)$$
$$= \{u : \mathbb{R}^N \to \mathbb{C},\ \partial_x^\alpha(e^{a\langle x\rangle}u(\cdot)), \in L^p(\mathbb{R}^N),\ |\alpha| \le r\}, \quad \text{if } r \in \mathbb{Z}_+,$$

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# Heat Kernel short-time asymptotics

Short-time asymptotic expansions well-known in literature:

- **Geodesic flow** ($L =$ Laplace-Beltrami operator):

$$\mathcal{G}_t(x,y) = \frac{e^{-\frac{d(x,y)^2}{4t}}}{(4\pi t)^{N/2}} \left( \mathcal{G}^{(0)}(x,y) + \mathcal{G}^{(1)}(x,y)t + \mathcal{G}^{(2)}(x,y)t^n + \dots \right),$$

  $d(x,y)$ geodesic distance (McKean-Singer, Greiner,..).

- **Parametrix** approximation (related to WKBJ)

$$\mathcal{G}^L(t,x,y) \sim \sum_{j\geq 0} t^{(j-n)/2} p_j\left(x, t^{-1/2}(x-y)\right) e^{\frac{-(x-y)^T A(x)^{-1}\cdot(x-y)}{4t}},$$

  $p_j(x,w)$ a polynomial of degree $j$ in $w$ (Melrose, Taylor, ...).

- **Hermite function** expansion (Y. Ait-Sahalia).

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# Implementation issues

- Our method is also based on a parametrix, but more easily implementable. It combines well with numerical methods to solve over large time intervals.
- Geodesic flow approximation is very accurate, but difficult to implement in practice. Except in special cases, geodesics must be computed numerically. Also, extension to time dependent coefficients not straightforward.
- Challenging to solve the PDE directly (unbounded domain, high dimensionality in certain problems, degeneracy of $L$)
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# Our expansion

- Based on Taylor expansion of *parabolic rescaling* $L^{s,z}$ of operator $L$:

$$L^{s,z} := \sum_{i,j=1}^{N} a_{ij}^{s,z}(x)\partial_i\partial_j + s\sum_{i=1}^{N} b_i^{s,z}(x)\partial_i + s^2 c^{s,z}(x),$$

$$f^{s,z}(t,x) := f(s^2 t, z + s(x-z)),$$

$z$ dilation center, $s$ dilation parameter (eventually, $s = \sqrt{t}$).

- Dilation center $z$ allowed to be a function of $x, y$ (may improve accuracy).
- Taylor expansion coupled with time-ordered perturbative expansion via Duhamel's principle.

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## Definition

$z : \mathbb{R}^{2N} \to \mathbb{R}^N$ is **admissible** if $z(x,x) = x$, and all derivatives are bounded. Ex: $z = x$, $z = \frac{x+y}{2}$.

For each $\mu \in \mathbb{Z}_+$ and $z = z(x,y)$ admissible, let:

$$\mathcal{G}_t^{[\mu,z]}(x,y) := t^{-N/2} \sum_{\ell=0}^{\mu} t^{\ell/2}\, \mathfrak{P}^\ell\Big(z, z + \frac{x-z}{t^{1/2}}, z + \frac{y-z}{t^{1/2}}\Big) \cdot \frac{1}{\sqrt{4\pi t^N \det(A(z))}} e^{-\frac{(x-y)^T A^{-1}(z)(x-y)}{4t}}\Big),$$

where $\mathfrak{P}^\ell(z,x,y) = \sum_{|\alpha|\le \ell, \beta \le 3\ell} a_{\alpha,\beta}(z)(x-z)^\alpha (x-y)^\beta$,

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# Main Result

## Theorem

*Let $\mu \in \mathbb{Z}_+$, $z = z(x, y)$ an admissible function. Then, $\exists\ a_{\alpha,\beta}$ explicitly computable such that*

$$e^{t\,L} f(x) = \int_{\mathbb{R}^N} \mathcal{G}_t^{[\mu,z]}(x, y) f(y) dy + t^{(\mu+1)/2} \mathcal{E}_t^{[\mu,z]} f(x).$$

*where, for any $a \in \mathbb{R}$, $m \in \mathbb{R}^+$, $1 < p < \infty$, $k \in \mathbb{Z}_+$,*

$$\|\mathcal{E}_t^{[\mu,z]} f\|_{W^{m+k,p}} \leq C t^{-k/2} \|f\|_{W^{m,p}},$$

$\mathcal{G}_t^{[\mu,z]}(x, y)$ is the $\mu$**th-order approximate kernel** for the solution operator $e^{t\,L}$. $\mathcal{E}_t^{[\mu,z]}$ is the **error** operator.

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# Some remarks

- Expansion agrees with usual parametrix if $z = x$ and $L$ time independent. Can optimize choice of $z(x, y)$ (work in progress).
- When $z = x$, our construction is equivalent to Taylor's expanding the Green's function.
- Error estimates are global on $\mathbb{R}^N$ (generalize to *non-compact, complete* manifolds).
- In 1D, solution has closed form in term of Error Functions if initial data is piece-wise polynomial (e.g. pricing of contingent claims).

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# Proof - Duhamel's Formula

By Duhamel's principle, reduce to $\partial_t u - Lu = 0$.

$e^{tL}$ **analytic semigroup** on $W_a^{m,p}$ $\Rightarrow$

$$\|u(t)\|_{W_a^{r,p}} \le Ct^{(s-r)/2}\|f\|_{W_a^{s,p}}, \quad t \in (0,1].$$

$r \ge s$, $1 < p < \infty$, $C$ independent of $t$ and $a$ in bounded set.

The map

$$(0,\infty) \ni t \to e^{tL} \in \mathcal{B}(W_a^{s,p}, W_a^{r,p})$$

is smooth for any $s$, $r$.

Set $V = L - L_0$, $L_0$ given operator in the same class as $L$.

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Iterating Duhamel's give time-ordered (**Dyson**) expansion:

$$\begin{aligned} e^{tL} = \; & e^{tL_0} + t\int_{\Sigma_1} e^{t\tau_0 L_0} V e^{t\tau_1 L_0}\, d\tau \\ & + t^2 \int_{\Sigma_2} e^{t\tau_0 L_0} V e^{t\tau_1 L_0} V e^{t\tau_2 L_0}\, d\tau + \cdots + \\ & + t^d \int_{\Sigma_p} e^{t\tau_0 L_0} V e^{t\tau_1 L_0} \dots e^{t\tau_{d-1} L_0} V e^{t\tau_d L_0}\, d\tau \\ & + t^{d+1} \int_{\Sigma_{d+1}} e^{t\tau_0 L_0} V e^{t\tau_1 L_0} \dots e^{t\tau_d L_0} V e^{\tau_{d+1} L}\, d\tau, \end{aligned}$$

$\Sigma_k$ $k$-dim unit simplex, $d$ iteration level.
Integrals are Banach-valued Riemann integrals.

# Proof - Dilation and Taylor expansion

Given fixed point $z$ (*center*), $s > 0$, recall

$$L^{s,z} := \sum_{i,j=1}^{N} a_{ij}^{s,z}(x)\partial_i\partial_j + s\sum_{i=1}^{N} b_i^{s,z}(x)\partial_i + s^2 c^{s,z}(x) \quad \Rightarrow$$

$$\mathcal{G}_t^L(x,y) = s^{-N}\mathcal{G}_1^{L^{s,z}}(z+s^{-1}(x-z), z+s^{-1}(y-z)), \quad t = s^2.$$

Taylor expand $L^{s,z}$ to order $n = d$ in $s$ at 0:

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For each $\mu \leq n$, Dyson expansion becomes:

$$e^{L^{s,z}} = e^{L_0^z} + \sum_{\ell=1}^{\mu} s^\ell \Lambda_z^\ell + \sum_{\ell=\mu+1}^{\max(\ell,n+1)} s^\ell \Lambda_z^\ell = \sum_{\ell=0}^{\mu} s^\ell \Lambda_z^\ell + s^{\mu+1}\mathbb{E}_\mu^{s,z},$$

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Where, with $\Lambda^0_z = e^{L^z_0}$ set: $\Lambda^\ell_z := \sum_{\alpha\in\mathfrak{A}_\ell} \Lambda_{\alpha,z}$,

$\mathfrak{A}_{k,\ell} := \{\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_k) \in \mathbb{N}^k \ : \ |\alpha| = \ell\}$, $\mathfrak{A}_\ell := \bigcup_{k=1}^{\ell} \mathfrak{A}_{k,\ell}$.

And if $1 \le k \le n$,

$$\Lambda_{\alpha,z} := \int_{\Sigma_k} e^{\tau_0 L^z_0} L^z_{\alpha_1} e^{\tau_1 L^z_0} L^z_{\alpha_2} \cdots L^z_{\alpha_k} e^{\tau_k L^z_0} d\tau,$$

while if $k = n + 1$,

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# Proof - Commutators

If $\alpha \in \mathfrak{A}_\ell$, $L^z_\alpha$ differential operator of order $\ell + 2$ and degree $\ell$ polynomial coefficients (say $L^z_\alpha \in \mathcal{D}(\ell, \ell + 2)$).

Campbell-Baker-Hasdorff formula then gives:

$$e^{\theta L_0} L^z_\alpha = P_\alpha(\theta) e^{\theta L_0},$$

where $P_\alpha(\theta) = P_\alpha(L_0, L^z_\alpha; \theta, x, \partial) \in \mathcal{D}(\ell, \ell + 2)$ given by

$$P_\ell(\theta) := \sum_{k=0}^{\ell} \frac{\theta^k}{k!} \operatorname{ad}^k_{L_0}(L^z_\alpha)$$

# Proof - Commutators

If $\alpha \in \mathfrak{A}_\ell$, $L^z_\alpha$ differential operator of order $\ell + 2$ and degree $\ell$ polynomial coefficients (say $L^z_\alpha \in \mathcal{D}(\ell, \ell + 2)$).

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# Proof - Expansion revisited

For $\ell \leq n$, then have

$$\Lambda_\alpha^z = \int_{\Sigma_k} \prod_{i=1}^{k} P_{\alpha_i}(L_0^z, L_{\alpha_i}^z; 1-\sigma_i, x, \partial) d\sigma \, e^{L_0^z} := \mathcal{P}_\alpha(x, z, \partial) e^{L_0^z},$$

with

$$\mathcal{P}_\alpha(x, z, \partial) = \sum_{|\beta| \leq \ell} \sum_{|\gamma| \leq \ell + 2k} a_{\beta,\gamma}(z)(x-z)^\beta \partial_x^\gamma,$$

$a_{\beta,\gamma}$ smooth, bounded function.

Using explicit formula for $e^{L_0^z}(x, y)$, dilating back, substituting $z = z(x, y)$ gives the final formula for the approximation kernel.

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# Error Estimates

Let $z = z(x, y)$ admissible, $s = t^{1/2}$.
Two types of error terms in $\mathcal{E}_t^{[\mu,z]}$, operator with kernel:

$$s^{-N}\mathbb{E}_{\mu}^{s,z}(z + s^{-1}(x - z), z + s^{-1}(y - z)).$$

1. For $\mu < \ell \leq n$, operators $\mathcal{L}_{s,\ell}$ with kernel

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2. For $\ell \geq n + 1$, operators $\mathcal{L}_{s,\ell}$ with kernel

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1. For $\mu < \ell \leq n$, obtain error bounds *uniformly* in $s$ in $W_a^{r,p}$, for all $r \in \mathbb{R}$ by showing:

$$\mathcal{L}_{s,\ell} = b_s(x, \partial), \qquad b_s(x,\xi) = a_s(x, s\xi),$$

for some family of symbols $a_s$ bounded in $S^0_{1,0}$.

2. For $\ell \geq n+1$, use Riesz Lemma along with:

$$\partial_x^{\beta} \partial_z^{\beta'} \partial_y^{\beta''} \Lambda_z^{s,\ell}(x,y) = \langle \partial^{\beta} \delta_x \, , \partial_z^{\beta'} \Lambda_z^{s,\ell} \, \partial^{\beta''} \delta_y \rangle \Rightarrow$$

$$\|\mathcal{L}_{s,\ell}\|_{W^{r,p} \to W^{r,p}} \leq C_T \, t^{-r/2}, \qquad t \in (0, T].$$

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# Examples - 1D Formulas

Set $z = x$ and denote $\mathcal{G}_t^{\mu,z} =: \mathcal{G}_t^{\mu}$.

If $L(x) = \frac{1}{2}\Sigma(x)^2\partial_x^2 + \mu(x)\partial_x - \rho(x)$, then first-order approx kernel given by:

$$\mathcal{G}_t^{[1]}(x,y;z) =$$

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In pricing of contingent claims, initial data $u(x,0) = (x-K)_+$.

*h* is the claim *pay-off* and parameter $K$ is the *strike price*.

Then, first-order approx solution given by

$$u^{[1]}(t,x) = \frac{\sqrt{t}}{2\sqrt{2\pi}} e^{-\frac{(x-K)^2}{2\Sigma(x)^2 t}} \left(2\Sigma(x) - \Sigma'(x)(x-K)\right) + \frac{1}{2} \cdot \left( \operatorname{erf}\left( \frac{x-K}{\sqrt{2t\Sigma(x)}} \right) + 1 \right) (\mu(x)t + x - K)$$

Can easily compute 2nd-order approximation as well.

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# An example

Consider the **CEV** model (J.C. Cox, S. A. Ross) for pricing contingent claims:

$$L(x) = \frac{1}{2}\sigma^2 x^{2\beta}\partial_x^2 + rx\partial_x - r, \qquad \beta > 0.$$

Exact formula for $\beta = 1,\ 2/3$, otherwise series solution (Cox-Ross, D.Emanuel-J. MacBeth) in terms of Bessel's functions $\Rightarrow$ slow to compute.

Varadhan metric is complete if $\beta \geq 1$, our theorem applies. For $\beta = 1$, metric is Poincaré metric.

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Assume again initial data $u(x,0) = h(x) = (x-K)_+$.

Our 1st-order approximate solution for $z = x$:

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Compare exact formula with 1st-order approximation, when $\beta = 2/3$.

Closed-form solution avoid issues with numerical integration against Green's function.

In practice, important to approximate solution well near $x = K$.

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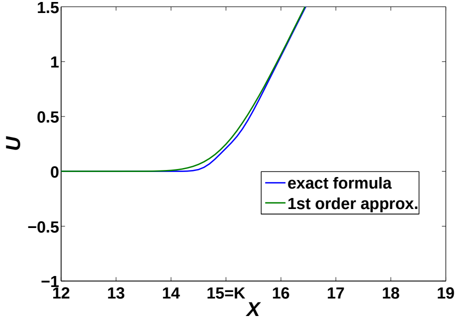
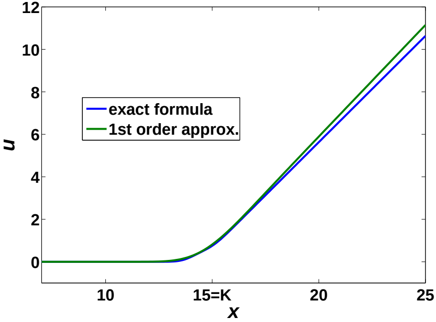
# Numerical Test - CEV Model

$\beta = \frac{2}{3}, K = 15, \sigma = 0.3, r = 0.1$ Error is $O(10^{-3})$




$t = 0.1$




$t = 0.5$

# Bootstrap to large time

Discuss only second-order approximation. Observe $e^{tL} = \left(e^{t/nL}\right)^n$.

Error in the second-order approx over time $t$ is $O(t)^{3/2})$.

Time step $t/n$ small if $n$ large, so error over one time step is small $\Rightarrow$ error $O((\frac{t}{n})^{3/2})$.

Denote by $\mathcal{G}^{[2]}_{t/n}$ the approximate solution operator over the time step $t/n$. Compare $e^{tL}$ with $\left(\mathcal{G}^{[2]}_{t/n}\right)^n$.

After $n$ steps, total error is

$$O((t/n)^{3/2}) \times n = O(t^{3/2}/\sqrt{n}) \to 0, \quad n \to \infty.$$

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- Error is not improved by bootstrap for first-order approximation (error is $O(t^{1/2})$.
- Prove rigorous error bound by using equivalent norm for which $e^{tL}$ is **contractive**.
- Neglect error from numerical quadrature at each time step. After first time step, no closed-form solutions available.
- Quadrature error negligible if space discretization fine enough. For $t > 0$ integrand is smooth, can use high-order methods away from $y = x$ (e.g. high-order Gaussian quadrature).
- Neglect error from truncation of domain (small if use compactly supported data).

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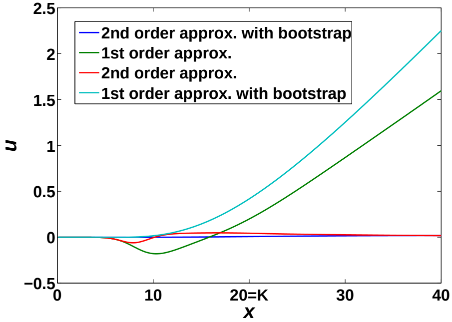
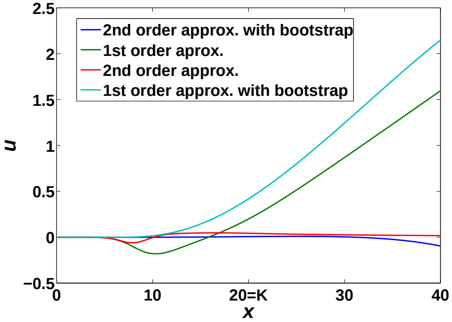
# Numerical test - CEV Model

$$\beta = 1,\ K = 20,\ \sigma = 0.3,\ r = 0.1, t = 1,\ n = 10$$

Error is $O(10^{-5})$ with bootstrap




Truncate at $x = 200$




Truncate at $x = 400$