# Convergence of Time-Stepping Deep Gradient Flow Methods

**Bachelier World Congress** 

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# Option pricing

$$\frac{\partial u}{\partial t} - \sum_{i,j=0}^{n} a^{ij} \frac{\partial^{2} u}{\partial x_{i} \partial x_{j}} - \sum_{i=0}^{n} b^{i} \frac{\partial u}{\partial x_{i}} + ru = 0$$
$$u(0,x) = \Phi(x)$$

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Can we solve this PDE using a neural network?

# Deep Galerkin Method <sup>1</sup>

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Minimize

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Issue: Taking second derivative makes training in high dimensions slow

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### Idea

Rewrite PDE as energy minimization problem

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- Only first order derivative
- No norm

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Split in symmetric and non-symmetric part

$$\frac{\partial u}{\partial t} = \sum_{i,j=0}^{n} a^{ij} \frac{\partial^{2} u}{\partial x_{i} \partial x_{j}} + \sum_{i=0}^{n} b^{i} \frac{\partial u}{\partial x_{i}} - ru$$

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$$= \sum_{i,j=0}^{n} \frac{\partial}{\partial x_{j}} \left( a^{ij} \frac{\partial u}{\partial x_{i}} \right) - \sum_{i,j=0}^{n} \frac{\partial a^{ij}}{\partial x_{j}} \frac{\partial u}{\partial x_{i}} + \sum_{i=0}^{n} b^{i} \frac{\partial u}{\partial x_{i}} - ru$$

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$$\begin{split} \frac{\partial u}{\partial t} &= \sum_{i,j=0}^{n} a^{ij} \frac{\partial^{2} u}{\partial x_{i} \partial x_{j}} + \sum_{i=0}^{n} b^{i} \frac{\partial u}{\partial x_{i}} - ru \\ &= \sum_{i,j=0}^{n} \frac{\partial}{\partial x_{j}} \left( a^{ij} \frac{\partial u}{\partial x_{i}} \right) - \sum_{i,j=0}^{n} \frac{\partial a^{ij}}{\partial x_{j}} \frac{\partial u}{\partial x_{i}} + \sum_{i=0}^{n} b^{i} \frac{\partial u}{\partial x_{i}} - ru \\ &= \sum_{i,j=0}^{n} \frac{\partial}{\partial x_{j}} \left( a^{ij} \frac{\partial u}{\partial x_{i}} \right) - \sum_{i=0}^{n} \left( \sum_{j=0}^{n} \frac{\partial a^{ij}}{\partial x_{j}} - b^{i} \right) \frac{\partial u}{\partial x_{i}} - ru \end{split}$$

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$$= \nabla \cdot (A \nabla u) - ru - F(u)$$

$$F(u) = \mathbf{b} \cdot \nabla u$$

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$$dS_t = rS_t dt + \sqrt{V_t} S_t dW_t \qquad S_0 > 0$$
  
$$dV_t = \kappa (\theta - V_t) dt + \eta \sqrt{V_t} dB_t \qquad V_0 > 0$$

$$\begin{split} dS_t &= rS_t dt + \sqrt{V_t} S_t dW_t & S_0 > 0 \\ dV_t &= \kappa (\theta - V_t) dt + \eta \sqrt{V_t} dB_t & V_0 > 0 \\ \frac{\partial u}{\partial t} &= rS \frac{\partial u}{\partial S} + \kappa (\theta - V) \frac{\partial u}{\partial V} + \frac{1}{2} S^2 V \frac{\partial^2 u}{\partial S^2} + \frac{1}{2} \eta^2 V \frac{\partial^2 u}{\partial V^2} + \rho \eta S V \frac{\partial^2 u}{\partial S \partial V} - ru \end{split}$$

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$$\begin{cases} u_t - \nabla \cdot (A\nabla u) + ru + F(u) = 0 & (t, \mathbf{x}) \in [0, T] \times \Omega \\ u(0, \mathbf{x}) = \Phi(\mathbf{x}) & \mathbf{x} \in \Omega \end{cases}$$

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• Divide [0, T] in intervals  $(t_{k-1}, t_k]$  with  $h = t_k - t_{k-1}$   $\frac{U^k - U^{k-1}}{h} - \nabla \cdot \left(A\nabla U^k\right) + rU^k + F\left(U^{k-1}\right) = 0$ 

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$$U^{0} = \Phi$$

### Theorem (Akrivis and Crouzeix 2004)

There exists a constant C independent of h and k such that

$$\max_{0 \le k \le N} \left\| u\left(t_{k}\right) - U^{k} \right\| \le Ch$$

$$\frac{U^k - U^{k-1}}{h} - \nabla \cdot \left(A\nabla U^k\right) + rU^k + F(U^{k-1}) = 0$$

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$$I^k(u) = \frac{1}{2} \left\| u - U^{k-1} \right\|^2 + h \int_{\Omega} \frac{1}{2} \left( (\nabla u)^T A\nabla u + ru^2 \right) + F\left(U^{k-1}\right) u dx$$

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The minimizer  $w_* \in \mathcal{H}^1_0\left(\mathbb{R}^d\right)$  of  $I^k$  is the unique solution  $U^k$ .

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$$i^{k}\left(\tau\right)=I^{k}\left(w_{*}+\tau v\right)$$

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Since  $w_*$  minimizes  $I^k$ ,  $\tau = 0$  minimizes  $i^k$ .

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$$0 = (i^{k})'(0)$$

$$= \int_{\mathbb{R}^{d}} ((w_{*} - U^{k-1}) + h(-\nabla \cdot (A\nabla w_{*}) + rw_{*} + F(U^{k-1}))) vdx.$$



### Definition (Activation function)

An activation function is a function  $\psi: \mathbb{R}^d \to \mathbb{R}$  such that  $\psi \in C_c^{\infty}(\mathbb{R}^d)$  and  $\int_{\mathbb{R}^d} \psi(x) \, \mathrm{d}x \neq 0$ .

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### Definition (Neural network)

$$C^{n}(\psi) = \left\{ \zeta(x) : \mathbb{R}^{d} \to \mathbb{R} : \zeta(x) = \sum_{i=1}^{n} \beta_{i} \psi(\alpha_{i} x + c_{i}) \right\},$$
$$C(\psi) = \bigcup_{n \ge 1} C^{n}(\psi)$$

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#### Theorem

 $\mathcal{C}(\psi)$  is dense in  $\mathcal{H}^1_0\left(\mathbb{R}^d\right)$ .

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Let  $w_m$  be a sequence in  $\mathcal{H}^1_0\left(\mathbb{R}^d\right)$  and  $w_*$  the minimizer of  $I^k$ .

$$\lim_{m\to\infty}\left\|w_{m}-w_{*}\right\|_{\mathcal{H}_{0}^{1}}=0\quad\iff\quad\lim_{m\to\infty}I^{k}\left(w_{m}\right)=I^{k}\left(w_{*}\right)$$

$$I^{k}(u) = \frac{1}{2} \left\| u - U^{k-1} \right\|^{2} + h \int_{\mathbb{R}^{d}} \frac{1}{2} \left( (\nabla u)^{T} A \nabla u + r u^{2} \right) + F \left( U^{k-1} \right) u dx$$

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$$=: \mathcal{L}^{k}(u) + \mathcal{G}^{k}(u),$$

$$\mathcal{L}^{k}(u) = \frac{1}{2} \| u \|^{2} + \frac{h}{2} \int_{\mathbb{R}^{d}} (\nabla u)^{T} A \nabla u + r u^{2} dx,$$

$$\mathcal{G}^{k}(u) = -\left\langle u, U^{k-1} \right\rangle + \frac{1}{2} \| U^{k-1} \|^{2} + h \int_{\mathbb{R}^{d}} F \left( U^{k-1} \right) u dx$$

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#### Proof.

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$$\iff w_m \rightharpoonup w_*. \text{ So } \mathcal{G}^n\left[w_m\right] \rightarrow \mathcal{G}^n\left[w_*\right].$$
 Since  $I^k\left(w_m\right) \rightarrow I^k\left(w_*\right), \ \mathcal{L}^k\left(w_m\right) \rightarrow \mathcal{L}^k\left(w_*\right).$ 

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$$\implies I^{k} \text{ is continuous.}$$

$$\iff w_{m} \rightharpoonup w_{*}. \text{ So } \mathcal{G}^{n}[w_{m}] \rightarrow \mathcal{G}^{n}[w_{*}].$$
Since  $I^{k}(w_{m}) \rightarrow I^{k}(w_{*}), \mathcal{L}^{k}(w_{m}) \rightarrow \mathcal{L}^{k}(w_{*}).$ 

$$\frac{1+hr}{2} \|w_{m} - w_{*}\|^{2} + \frac{h}{2} \|\sqrt{A}\nabla(w_{m} - w_{*})\|^{2} \rightarrow 0.$$

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$$\Rightarrow I^{k} \text{ is continuous.}$$

$$\Leftarrow w_{m} \rightharpoonup w_{*}. \text{ So } \mathcal{G}^{n} [w_{m}] \rightarrow \mathcal{G}^{n} [w_{*}].$$
Since  $I^{k} (w_{m}) \rightarrow I^{k} (w_{*}), \mathcal{L}^{k} (w_{m}) \rightarrow \mathcal{L}^{k} (w_{*}).$ 

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$$\|w_{m} - w_{*}\|_{\mathcal{H}_{0}^{1}} \rightarrow 0.$$

# Convergence when training

#### Neural network:

$$V_t^N\left(\theta^N;x\right) = V^N\left(\theta_t^N;x\right) = N^{-\delta} \sum_{i=1}^N \beta^i \psi\left(\alpha^i x + c^i\right),$$

$$\theta^{\textit{N}} = \left(\beta^{\textit{i}}, \alpha^{\textit{i}}, c^{\textit{i}}\right)_{\textit{i}=1}^{\textit{N}}, \, \tfrac{1}{2} < \delta < 1.$$

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$$\theta^{N} = (\beta^{i}, \alpha^{i}, c^{i})_{i=1}^{N}, \frac{1}{2} < \delta < 1.$$

$$V_t^N \stackrel{N \to \infty}{\longrightarrow} V_t \stackrel{t \to \infty}{\longrightarrow} w_*$$

## Gradient Descent

$$V^{N}\left(\theta^{N};x\right) = N^{-\delta} \sum_{i=1}^{N} \beta^{i} \psi\left(\alpha^{i} x + c^{i}\right),$$

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## **Gradient Descent**

$$\begin{split} V^N\left(\theta^N;x\right) &= N^{-\delta} \sum_{i=1}^N \beta^i \psi\left(\alpha^i x + c^i\right), \\ \theta^N &= \left(\beta^i,\alpha^i,c^i\right)_{i=1}^N, \ \frac{1}{2} < \delta < 1. \ \eta_N = N^{2\delta-1} \\ \frac{\mathrm{d}\theta^N_t}{\mathrm{d}t} &= -\eta_N \nabla_\theta I^k\left(V^N\left(\theta^N_t;x\right)\right) \end{split}$$

## Gradient Descent

$$\begin{split} V^{N}\left(\boldsymbol{\theta}^{N};\boldsymbol{x}\right) &= N^{-\delta} \sum_{i=1}^{N} \beta^{i} \psi\left(\alpha^{i} \boldsymbol{x} + \boldsymbol{c}^{i}\right), \\ \boldsymbol{\theta}^{N} &= \left(\beta^{i}, \alpha^{i}, \boldsymbol{c}^{i}\right)_{i=1}^{N}, \ \frac{1}{2} < \delta < 1. \ \eta_{N} = N^{2\delta - 1} \\ &\qquad \qquad \frac{\mathrm{d}\boldsymbol{\theta}_{t}^{N}}{\mathrm{d}t} = -\eta_{N} \nabla_{\boldsymbol{\theta}} \boldsymbol{I}^{k} \left(\boldsymbol{V}^{N}\left(\boldsymbol{\theta}_{t}^{N}; \boldsymbol{x}\right)\right) \\ &\qquad \qquad \frac{\mathrm{d}\boldsymbol{V}_{t}^{N}\left(\boldsymbol{x}\right)}{\mathrm{d}t} = \nabla_{\boldsymbol{\theta}} \boldsymbol{V}^{N}\left(\boldsymbol{\theta}_{t}^{N}; \boldsymbol{x}\right) \cdot \frac{\mathrm{d}\boldsymbol{\theta}_{t}^{N}}{\mathrm{d}t} \\ &= -\eta_{N} \nabla_{\boldsymbol{\theta}} \boldsymbol{V}^{N}\left(\boldsymbol{\theta}_{t}^{N}; \boldsymbol{x}\right) \cdot \nabla_{\boldsymbol{\theta}} \boldsymbol{I}^{k} \left(\boldsymbol{V}^{N}\left(\boldsymbol{\theta}_{t}^{N}; \boldsymbol{x}\right)\right) \end{split}$$

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## Convergence in neurons

$$\frac{\mathrm{d}V_{t}^{N}(x)}{\mathrm{d}t} = -\eta_{N}\nabla_{\theta}V^{N}\left(\theta_{t}^{N};x\right)\cdot\nabla_{\theta}I^{k}\left(V^{N}\left(\theta_{t}^{N};x\right)\right)$$

## Convergence in neurons

$$\begin{split} \frac{\mathrm{d}V_{t}^{N}\left(x\right)}{\mathrm{d}t} &= -\eta_{N}\nabla_{\theta}V^{N}\left(\theta_{t}^{N};x\right)\cdot\nabla_{\theta}I^{k}\left(V^{N}\left(\theta_{t}^{N};x\right)\right) \\ &= -\left\langle \mathcal{D}I^{k}\left(V_{t}^{N}\right),Z_{t}^{N}\left(x,.\right)\right\rangle_{\mathcal{H}_{0}^{1}} \end{split}$$

$$Z_{t}^{N}(x,y) = N^{-1} \sum_{i=1}^{N} \nabla_{\beta,\alpha,c} \beta_{t}^{i} \psi \left( \alpha_{t}^{i} x + c_{t}^{i} \right) \cdot \nabla_{\beta,\alpha,c} \beta_{t}^{i} \psi \left( \alpha_{t}^{i} y + c_{t}^{i} \right)$$

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## Convergence in neurons

$$\begin{split} \frac{\mathrm{d}V_{t}^{N}\left(x\right)}{\mathrm{d}t} &= -\eta_{N}\nabla_{\theta}V^{N}\left(\theta_{t}^{N};x\right)\cdot\nabla_{\theta}I^{k}\left(V^{N}\left(\theta_{t}^{N};x\right)\right)\\ &= -\left\langle\mathcal{D}I^{k}\left(V_{t}^{N}\right),Z_{t}^{N}\left(x,.\right)\right\rangle_{\mathcal{H}_{0}^{1}}\\ \frac{\mathrm{d}V_{t}\left(x\right)}{\mathrm{d}t} &= -\left\langle\mathcal{D}I^{k}\left(V_{t}\right),Z\left(x,.\right)\right\rangle_{\mathcal{H}_{0}^{1}}\\ Z_{t}^{N}\left(x,y\right) &= N^{-1}\sum_{i=1}^{N}\nabla_{\beta,\alpha,c}\beta_{t}^{i}\psi\left(\alpha_{t}^{i}x+c_{t}^{i}\right)\cdot\nabla_{\beta,\alpha,c}\beta_{t}^{i}\psi\left(\alpha_{t}^{i}y+c_{t}^{i}\right)\\ Z\left(x,y\right) &= \mathbb{E}\left[\nabla_{\beta,\alpha,c}\beta_{0}^{1}\psi\left(\alpha_{0}^{1}x+c_{0}^{1}\right)\cdot\nabla_{\beta,\alpha,c}\beta_{0}^{1}\psi\left(\alpha_{0}^{1}y+c_{0}^{1}\right)\right] \end{split}$$

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$$\begin{split} \frac{\mathrm{d}V_{t}^{N}\left(x\right)}{\mathrm{d}t} &= -\left\langle \mathcal{D}I^{k}\left(V_{t}^{N}\right), Z_{t}^{N}\left(x,.\right)\right\rangle_{\mathcal{H}_{0}^{1}} \\ \frac{\mathrm{d}V_{t}\left(x\right)}{\mathrm{d}t} &= -\left\langle \mathcal{D}I^{k}\left(V_{t}\right), Z\left(x,.\right)\right\rangle_{\mathcal{H}_{0}^{1}} \\ Z_{t}^{N}\left(x,y\right) &= N^{-1}\sum_{i=1}^{N}\nabla_{\beta,\alpha,c}\beta_{t}^{i}\psi\left(\alpha_{t}^{i,N}x + c_{t}^{i,N}\right) \cdot \nabla_{\beta,\alpha,c}\beta_{t}^{i}\psi\left(\alpha_{t}^{i,N}y + c_{t}^{i,N}\right) \\ Z\left(x,y\right) &= \mathbb{E}\left[\nabla_{\beta,\alpha,c}\beta_{0}^{1}\psi\left(\alpha_{0}^{1}x + c_{0}^{1}\right) \cdot \nabla_{\beta,\alpha,c}\beta_{0}^{1}\psi\left(\alpha_{0}^{1}y + c_{0}^{1}\right)\right] \end{split}$$

$$\frac{\mathrm{d}V_{t}^{N}(x)}{\mathrm{d}t} = -\left\langle \mathcal{D}I^{k}\left(V_{t}^{N}\right), Z_{t}^{N}(x,.)\right\rangle_{\mathcal{H}_{0}^{1}}$$
$$\frac{\mathrm{d}V_{t}(x)}{\mathrm{d}t} = -\left\langle \mathcal{D}I^{k}\left(V_{t}\right), Z(x,.)\right\rangle_{\mathcal{H}_{0}^{1}}$$

$$Z_{t}^{N}(x,y) = N^{-1} \sum_{i=1}^{N} \nabla_{\beta,\alpha,c} \beta_{t}^{i} \psi \left( \alpha_{t}^{i,N} x + c_{t}^{i,N} \right) \cdot \nabla_{\beta,\alpha,c} \beta_{t}^{i} \psi \left( \alpha_{t}^{i,N} y + c_{t}^{i,N} \right)$$
$$Z(x,y) = \mathbb{E} \left[ \nabla_{\beta,\alpha,c} \beta_{0}^{1} \psi \left( \alpha_{0}^{1} x + c_{0}^{1} \right) \cdot \nabla_{\beta,\alpha,c} \beta_{0}^{1} \psi \left( \alpha_{0}^{1} y + c_{0}^{1} \right) \right]$$

#### Theorem

For any T > 0,

$$\sup_{0 \leq t \leq T} \mathbb{E} \left[ \left\| V_t^N - V_t \right\|_{\mathcal{H}_0^1} \right] \overset{N \to \infty}{\longrightarrow} 0.$$

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#### Theorem

$$\lim_{t\to\infty}\|V_t-w_*\|_{\mathcal{H}^1_0}=0.$$

$$\frac{\mathrm{d}V_{t}\left(x\right)}{\mathrm{d}t}=-\left\langle \mathcal{D}I^{k}\left(V_{t}\right),Z\left(x,.\right)\right\rangle _{\mathcal{H}_{0}^{1}}$$

#### **Theorem**

$$\lim_{t\to\infty}\|V_t-w_*\|_{\mathcal{H}^1_0}=0.$$

$$\begin{split} \frac{\mathrm{d}V_{t}\left(x\right)}{\mathrm{d}t} &= -\left\langle \mathcal{D}I^{k}\left(V_{t}\right), Z\left(x,.\right)\right\rangle_{\mathcal{H}_{0}^{1}} \\ \frac{\mathrm{d}\left(V_{t}-w_{*}\right)\left(x\right)}{\mathrm{d}t} &= -\left\langle \mathcal{D}I^{k}\left(V_{t}-w_{*}+w_{*}\right), Z\left(x,.\right)\right\rangle_{\mathcal{H}_{0}^{1}} \\ &= -\tilde{\mathcal{T}}\left(V_{t}-w_{*}\right)\!\left(x\right) \end{split}$$

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Proof: 
$$\lim_{t\to\infty} \|V_t - w_*\|_{\mathcal{H}^1_0} = 0.$$

 $\tilde{\mathcal{T}}$  is a self-adjoint, positive definite trace class operator. Spectral decomposition:

$$\tilde{\mathcal{T}}(\tilde{e}_i) = \lambda_i \tilde{e}_i,$$

 $\lambda_1 \geq \lambda_2 \geq ... > 0$ , orthogonal basis  $\{\tilde{e}_i\}_{i=1}^{\infty}$ .

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Proof:  $\lim_{t\to\infty} \|V_t - w_*\|_{\mathcal{H}_0^1} = 0.$ 

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$$egin{aligned} rac{\mathrm{d} h_t^i}{\mathrm{d} t} := & rac{\langle \mathrm{d} (V_t - w_*), ilde{e}_i 
angle}{\mathrm{d} t} = - \left\langle ilde{\mathcal{T}} (V_t - w_*), ilde{e}_i 
ight
angle = - \left\langle V_t - w_*, ilde{\mathcal{T}} ( ilde{e}_i) 
ight
angle \\ = - \lambda_i h_t^i. \end{aligned}$$

Proof:  $\lim_{t\to\infty} \|V_t - w_*\|_{\mathcal{H}_0^1} = 0.$ 

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$$h_t^i = e^{-\lambda_i t} h_0^i.$$

Proof:  $\lim_{t\to\infty} \|V_t - w_*\|_{\mathcal{H}_0^1} = 0.$ 

 $\tilde{\mathcal{T}}$  is a self-adjoint, positive definite trace class operator. Spectral decomposition:

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ight
angle = - \left\langle V_{t} - w_{*}, ilde{\mathcal{T}}( ilde{e}_{i}) 
ight
angle \\ = - \lambda_{i} h_{t}^{i}. \end{aligned}$$

 $h_t^i = e^{-\lambda_i t} h_0^i$ . Parseval's identity:

$$\|V_t - w_*\|^2 = \sum_{i=1}^{\infty} (h_t^i)^2 = \sum_{i=1}^{\infty} e^{-2\lambda_i t} (h_0^i)^2 \stackrel{t \to \infty}{\longrightarrow} 0.$$

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# Convergence of Time-Stepping Deep Gradient Flow Methods

Bachelier World Congress

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