

Fréchet derivatives under various parameterizations  
using chain rule  
for LEGO module m\_parameterization.f90

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# Overview

Physical meaning of symbols uniformly used in this code:

$v_p$	P-wave velocity
$v_s$	S-wave velocity
$sp = 1/v_p$	P-wave slowness
$sps = v_s/v_p$	inv $V_p$ - $V_s$ ratio
$ip = v_p \cdot \rho$	P-wave (acoustic) impedance
$\rho$	density
$kpa = \rho \cdot v_p^2$	bulk modulus
$lda = \rho \cdot (v_p^2 - 2v_s^2)$	1st Lamé parameter
$\mu = \rho \cdot v_s^2$	2nd Lamé parameter, shear modulus

## Considered parameterizations

SITUATION	PARAMETERIZATION	ALLOWED PARAMETERS
WaveEquation	moduli-density	kpa (or lda mu) rho
canonical models	velocities-density	vp vs rho
seismic	velocities-impedance	vp vs ip
tomography	slowness-density	sp sps rho
optimization	can be any of above	—

## Source-Destination trilogy:



- ▶ model m  $\rightarrow$  WaveEq lm depending on field.
- ▶ WaveEq produces gkpa (or glda, gmu) and grho under moduli-density parameterization.
- ▶ then m\_parameterization.f90 converts them to another parameterization for optim x,g, which can be any of parameterization

## ACTIVE versus PASSIVE

- ▶ Active parameters will be converted to  $\text{optim } x$  via feature scaling (e.g.  $(\text{par} - \text{par\_min}) / (\text{par\_max} - \text{par\_min})$ ), and will be updated by optimization methods.
  - ▶ Mono-parameter inversion: 1 active parameter.
  - ▶ Multi-parameter inversion:  $> 1$  active parameters.
    - ▶ Scaling in `m_linesearch.f90` depends only on the 1st active parameters (no matter of it's velocity or not).
    - ▶ Output of inversion results has same sequence of active parameters listed in `setup.in`
- ▶ Passive parameters will NOT be converted to  $\text{optim } x$ , and will NOT be updated by optimization methods.
- ▶ However, they may still be updated according to user-specified empirical law (e.g. Gardner), which serves as hard constraints between parameters.
  - ▶ User has to modified the code where necessary to insert such a law as symbolic computation is not straightforward in fortran
  - ▶ Such a law may change the  $\text{optim } g$  for active parameters.

velocities-density

velocities-impedance

slowness-density

# PARAMETERIZATION velocities-density

isotropic ACooustic

$$\begin{aligned} & \left\{ \begin{array}{l} \kappa = \rho V_P^2 \\ \rho_0 = \rho \end{array} \right. \\ \nabla_{V_P} &= \nabla_{\kappa} \frac{\partial \kappa}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\ &= \nabla_{\kappa} 2\rho V_P \\ \nabla_{\rho} &= \nabla_{\kappa} \frac{\partial \kappa}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho} \\ &= \nabla_{\kappa} V_P^2 + \nabla_{\rho_0} \end{aligned}$$

$$\begin{aligned} & \left\{ \begin{array}{l} V_P = \sqrt{\frac{\kappa}{\rho_0}} \\ \rho = \rho_0 \end{array} \right. \\ \nabla_{\kappa} &= \nabla_{V_P} \frac{\partial V_P}{\partial \kappa} + \nabla_{\rho} \frac{\partial \rho}{\partial \kappa} \\ &= \nabla_{V_P} \frac{1}{2\rho_0} \sqrt{\frac{\rho_0}{\kappa}} \\ &= \nabla_{V_P} 0.5\rho_0^{-0.5} \kappa^{-0.5} \\ \nabla_{\rho_0} &= \nabla_{V_P} \frac{\partial V_P}{\partial \rho_0} + \nabla_{\rho} \frac{\partial \rho}{\partial \rho_0} \\ &= \nabla_{V_P} \left( -\frac{\kappa}{2\rho_0^2} \sqrt{\frac{\rho_0}{\kappa}} \right) + \nabla_{\rho} \\ &= \nabla_{V_P} \left( -0.5\rho_0^{-1.5} \kappa^{0.5} \right) + \nabla_{\rho} \end{aligned}$$

# PARAMETERIZATION velocities-density + PASSIVE gardner

isotropic ACOUSTIC

$$\rho = aV_P^b$$

$$\left\{ \begin{array}{l} \kappa = \rho V_P^2 = aV_P^{b+2} \\ \rho_0 = \rho = aV_P^b \end{array} \right.$$

$$V_P = \left( \frac{\kappa}{a} \right)^{\frac{1}{b+2}}$$

$$\begin{aligned} \nabla_{V_P} &= \nabla_{\kappa} \frac{\partial \kappa}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\ &= \nabla_{\kappa} a(b+2)V_P^{b+1} + \nabla_{\rho_0} abV_P^{b-1} \\ &= \left( \nabla_{\kappa} \frac{b+2}{b} V_P^2 + \nabla_{\rho_0} \right) abV_P^{b-1} \end{aligned}$$

$$\begin{aligned} \nabla_{\kappa} &= \nabla_{V_P} \frac{\partial V_P}{\partial \kappa} \\ &= \nabla_{V_P} \frac{1}{a(b+2)} \left( \frac{\kappa}{a} \right)^{-\frac{b+1}{b+2}} \end{aligned}$$

# PARAMETERIZATION velocities-density

isotropic P-SV

$$\left\{ \begin{array}{l} \lambda = \rho(V_P^2 - 2V_S^2) \\ \mu = \rho V_S^2 \\ \rho_0 = \rho \end{array} \right.$$

$$\nabla_{V_P} = \nabla_\lambda \frac{\partial \lambda}{\partial V_P} + \nabla_\mu \frac{\partial \mu}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P}$$

$$= \nabla_\lambda 2\rho V_P$$

$$\nabla_{V_S} = \nabla_\lambda \frac{\partial \lambda}{\partial V_S} + \nabla_\mu \frac{\partial \mu}{\partial V_S} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_S}$$

$$= \nabla_\lambda (-4)\rho V_S + \nabla_\mu 2\rho V_S$$

$$= (-2\nabla_\lambda + \nabla_\mu) 2\rho V_S$$

$$\nabla_\rho = \nabla_\lambda \frac{\partial \lambda}{\partial \rho} + \nabla_\mu \frac{\partial \mu}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho}$$

$$= \nabla_\lambda (V_P^2 - 2V_S^2) + \nabla_\mu V_S^2 + \nabla_{\rho_0}$$

$$= \nabla_\lambda V_P^2 + (-2\nabla_\lambda + \nabla_\mu) V_S^2 + \nabla_{\rho_0}$$

$$\left\{ \begin{array}{l} V_P = \sqrt{\frac{\lambda + 2\mu}{\rho_0}} \\ V_S = \sqrt{\frac{\mu}{\rho_0}} \\ \rho = \rho_0 \end{array} \right.$$

$$\nabla_{V_P} \frac{\partial V_P}{\partial \lambda} + \nabla_{V_S} \frac{\partial V_S}{\partial \lambda} + \nabla_\rho \frac{\partial \rho}{\partial \lambda}$$

$$= \dots$$

$$\nabla_{V_P} \frac{\partial V_P}{\partial \mu} + \nabla_{V_S} \frac{\partial V_S}{\partial \mu} + \nabla_\rho \frac{\partial \rho}{\partial \mu}$$

$$= \dots$$

$$\nabla_{V_P} \frac{\partial V_P}{\partial \rho_0} + \nabla_{V_S} \frac{\partial V_S}{\partial \rho_0} + \nabla_\rho \frac{\partial \rho}{\partial \rho_0}$$

$$= \dots$$



# PARAMETERIZATION velocities-density + PASSIVE gardner

isotropic P-SV

$$\rho = aV_P^b$$

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = aV_P^{b+2} - 2aV_P^bV_S^2 \\ \mu = \rho V_S^2 = aV_P^bV_S^2 \\ \rho_0 = \rho = aV_P^b \end{cases}$$

$$\begin{aligned} \nabla_{V_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_P} + \nabla_\mu \frac{\partial \mu}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\ &= \nabla_\lambda \left( a(b+2)V_P^{b+1} - 2abV_P^{b-1}V_S^2 \right) + \nabla_\mu abV_P^{b-1}V_S^2 + \nabla_{\rho_0} abV_P^{b-1} \\ &= \left( \nabla_\lambda \left( \frac{b+2}{b}V_P^2 - 2V_S^2 \right) + \nabla_\mu V_S^2 + \nabla_{\rho_0} \right) abV_P^{b-1} \\ &= \left( \nabla_\lambda \frac{b+2}{b}V_P^2 + (-2\nabla_\lambda + \nabla_\mu)V_S^2 + \nabla_{\rho_0} \right) abV_P^{b-1} \\ \nabla_{V_S} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_S} + \nabla_\mu \frac{\partial \mu}{\partial V_S} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_S} \\ &= \nabla_\lambda (-4aV_P^bV_S) + \nabla_\mu 2aV_P^bV_S \\ &= (-2\nabla_\lambda + \nabla_\mu) 2aV_P^bV_S \end{aligned}$$

velocities-density

velocities-impedance

slowness-density

# PARAMETERIZATION velocities-impedance

isotropic ACooustic

$$I_P = V_P \rho$$

$$\begin{cases} \kappa = \rho V_P^2 = V_P I_P \\ \rho_0 = \rho = \frac{I_P}{V_P} \end{cases}$$

$$\begin{aligned} \nabla_{V_P} &= \nabla_{\kappa} \frac{\partial \kappa}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\ &= \nabla_{\kappa} I_P + \nabla_{\rho_0} (-I_P V_P^{-2}) \\ &= \left( \nabla_{\kappa} - \nabla_{\rho_0} V_P^{-2} \right) V_P \rho \end{aligned}$$

$$\begin{aligned} \nabla_{I_P} &= \nabla_{\kappa} \frac{\partial \kappa}{\partial I_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial I_P} \\ &= \nabla_{\kappa} V_P + \nabla_{\rho_0} V_P^{-1} \end{aligned}$$

$$\begin{cases} V_P = \sqrt{\frac{\kappa}{\rho_0}} \\ I_P = \sqrt{\kappa \rho_0} \end{cases}$$

$$\begin{aligned} \nabla_{\kappa} &= \nabla_{V_P} \frac{\partial V_P}{\partial \kappa} + \nabla_{I_P} \frac{\partial I_P}{\partial \kappa} \\ &= \nabla_{V_P} \frac{1}{2\rho_0} \sqrt{\frac{\rho_0}{\kappa}} + \nabla_{I_P} \frac{\rho_0}{2\sqrt{\kappa\rho_0}} \\ &= \nabla_{V_P} 0.5\rho_0^{-0.5}\kappa^{-0.5} + \nabla_{I_P} 0.5\rho_0^{0.5}\kappa^{-0.5} \\ &= (\nabla_{V_P} + \nabla_{I_P}\rho_0) 0.5\rho_0^{-0.5}\kappa^{-0.5} \\ \nabla_{\rho_0} &= \nabla_{V_P} \frac{\partial V_P}{\partial \rho_0} + \nabla_{I_P} \frac{\partial I_P}{\partial \rho_0} \\ &= \nabla_{V_P} \frac{-\kappa}{2\rho_0^2} \sqrt{\frac{\rho_0}{\kappa}} + \nabla_{I_P} \frac{\kappa}{2\sqrt{\kappa\rho_0}} \\ &= \nabla_{V_P} (-0.5)\rho_0^{-1.5}\kappa^{0.5} + \nabla_{I_P} 0.5\rho_0^{-0.5}\kappa^{0.5} \\ &= \left( -\nabla_{V_P}\rho_0^{-1} + \nabla_{I_P} \right) 0.5\rho_0^{-0.5}\kappa^{0.5} \end{aligned}$$

# PARAMETERIZATION velocities-impedance

isotropic P-SV

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = V_P I_P - \frac{2V_S^2 I_P}{V_P} \\ \mu = \rho V_S^2 = \frac{V_S^2 I_P}{V_P} \\ \rho_0 = \rho = \frac{I_P}{V_P} \end{cases}$$

$$\begin{aligned} \nabla_{V_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_P} + \nabla_\mu \frac{\partial \mu}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\ &= \nabla_\lambda \left( I_P + \frac{2V_S^2 I_P}{V_P^2} \right) + \nabla_\mu \left( -\frac{V_S^2 I_P}{V_P^2} \right) + \nabla_{\rho_0} \left( -\frac{I_P}{V_P^2} \right) \\ &= \left( \nabla_\lambda (V_P^2 + 2V_S^2) - \nabla_\mu V_S^2 - \nabla_{\rho_0} \right) \frac{I_P}{V_P^2} \\ &= \left( \nabla_\lambda V_P^2 + (2\nabla_\lambda - \nabla_\mu) V_S^2 - \nabla_{\rho_0} \right) \frac{\rho}{V_P} \\ \nabla_{V_S} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_S} + \nabla_\mu \frac{\partial \mu}{\partial V_S} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_S} \\ &= \nabla_\lambda \frac{-4V_S I_P}{V_P} + \nabla_\mu \frac{2V_S I_P}{V_P} \\ &= (-2\nabla_\lambda + \nabla_\mu) \frac{2V_S I_P}{V_P} \\ &= (-2\nabla_\lambda + \nabla_\mu) 2V_S \rho \end{aligned}$$

# PARAMETERIZATION velocities-impedance

isotropic P-SV *continued*

$$\left\{ \begin{array}{l} \lambda = \rho(V_P^2 - 2V_S^2) = V_P I_P - \frac{2V_S^2 I_P}{V_P} \\ \mu = \rho V_S^2 = \frac{V_S^2 I_P}{V_P} \\ \rho_0 = \rho = \frac{I_P}{V_P} \end{array} \right.$$

$$\begin{aligned} \nabla_{I_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial I_P} + \nabla_\mu \frac{\partial \mu}{\partial I_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial I_P} \\ &= \nabla_\lambda \left( V_P - \frac{2V_S^2}{V_P} \right) + \nabla_\mu \frac{V_S^2}{V_P} + \nabla_{\rho_0} \frac{1}{V_P} \\ &= \left( \nabla_\lambda (V_P^2 - 2V_S^2) + \nabla_\mu V_S^2 + \nabla_{\rho_0} \right) \frac{1}{V_P} \\ &= \left( \nabla_\lambda V_P^2 + (-2\nabla_\lambda + \nabla_\mu) V_S^2 + \nabla_{\rho_0} \right) \frac{1}{V_P} \end{aligned}$$

velocities-density

velocities-impedance

slowness-density

# PARAMETERIZATION slowness-density

isotropic ACooustic

$$S_P = 1/V_P$$

$$\begin{cases} \kappa = \rho V_P^2 = \rho S_P^{-2} \\ \rho_0 = \rho \end{cases}$$

$$\begin{aligned} \nabla_{S_P} &= \nabla_{\kappa} \frac{\partial \kappa}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P} \\ &= \nabla_{\kappa} (-2\rho S_P^{-3}) \end{aligned}$$

$$\begin{aligned} \nabla_{\rho} &= \nabla_{\kappa} \frac{\partial \kappa}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho} \\ &= \nabla_{\kappa} S_P^{-2} + \nabla_{\rho_0} \end{aligned}$$

$$\begin{cases} S_P = \sqrt{\frac{\rho_0}{\kappa}} \\ \rho = \rho_0 \end{cases}$$

$$\begin{aligned} \nabla_{\kappa} &= \nabla_{S_P} \frac{\partial S_P}{\partial \kappa} + \nabla_{\rho} \frac{\partial \rho}{\partial \kappa} \\ &= \nabla_{S_P} \left( \frac{1}{2} \sqrt{\frac{\kappa}{\rho_0}} \frac{-\rho_0}{\kappa^2} \right) \end{aligned}$$

$$= \nabla_{S_P} (-0.5) \rho_0^{0.5} \kappa^{-1.5}$$

$$\begin{aligned} \nabla_{\rho_0} &= \nabla_{S_P} \frac{\partial S_P}{\partial \rho_0} + \nabla_{\rho} \frac{\partial \rho}{\partial \rho_0} \\ &= \nabla_{S_P} \left( \frac{1}{2} \sqrt{\frac{\kappa}{\rho_0}} \frac{1}{\kappa} \right) + \nabla_{\rho} \\ &= \nabla_{S_P} 0.5 \rho_0^{-0.5} \kappa^{-0.5} + \nabla_{\rho} \end{aligned}$$

# PARAMETERIZATION slowness-density + PASSIVE gardner

isotropic ACooustic

$$\rho = aS_P^{-b}$$

$$\left\{ \begin{array}{l} \kappa = \rho V_P^2 = aS_P^{-b-2} \\ \rho_0 = \rho = aS_P^{-b} \end{array} \right.$$

$$S_P = \left( \frac{\kappa}{a} \right)^{-\frac{1}{b+2}}$$

$$\begin{aligned} \nabla_{S_P} &= \nabla_{\kappa} \frac{\partial \kappa}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P} \\ &= \nabla_{\kappa} a(-b-2)S_P^{-b-3} \\ &\quad + \nabla_{\rho_0} (-ab)S_P^{-b-1} \\ &= -\left( \nabla_{\kappa} a(b+2) + \nabla_{\rho_0} abS_P^2 \right) S_P^{-b-3} \end{aligned}$$

$$\begin{aligned} \nabla_{\kappa} &= \nabla_{S_P} \frac{\partial S_P}{\partial \kappa} \\ &= \nabla_{S_P} \frac{-1}{a(b+2)} \left( \frac{\kappa}{a} \right)^{-\frac{b+3}{b+2}} \end{aligned}$$



# PARAMETERIZATION slowness-density

isotropic P-SV

$$S_{PS} = V_S/V_P = V_S S_P$$

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = \rho S_P^{-2}(1 - 2S_{PS}^2) \\ \mu = \rho V_S^2 = \rho(S_{PS}/S_P)^2 \\ \rho_0 = \rho \end{cases}$$

$$\begin{aligned} \nabla_{S_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial S_P} + \nabla_\mu \frac{\partial \mu}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P} \\ &= \nabla_\lambda \rho (-2) S_P^{-3} (1 - 2S_{PS}^2) + \nabla_\mu \rho S_{PS}^2 (-2) S_P^{-3} \\ &= \left( \nabla_\lambda (1 - 2S_{PS}^2) + \nabla_\mu S_{PS}^2 \right) (-2) \rho S_P^{-3} \end{aligned}$$

$$\begin{aligned} \nabla_{S_{PS}} &= \nabla_\lambda \frac{\partial \lambda}{\partial S_{PS}} + \nabla_\mu \frac{\partial \mu}{\partial S_{PS}} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_{PS}} \\ &= \nabla_\lambda \rho S_P^{-2} (-4) S_{PS} + \nabla_\mu 2\rho S_{PS}/S_P^2 \\ &= (-\nabla_\lambda 2 + \nabla_\mu) 2\rho S_{PS} S_P^{-2} \end{aligned}$$

$$\begin{aligned} \nabla_\rho &= \nabla_\lambda \frac{\partial \lambda}{\partial \rho} + \nabla_\mu \frac{\partial \mu}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho} \\ &= \nabla_\lambda S_P^{-2} (1 - 2S_{PS}^2) + \nabla_\mu (S_{PS}/S_P)^2 + \nabla_{\rho_0} \\ &= \left( \nabla_\lambda (1 - 2S_{PS}^2) + \nabla_\mu S_{PS} \right) S_P^{-2} + \nabla_{\rho_0} \end{aligned}$$

# PARAMETERIZATION slowness-density + PASSIVE gardner

isotropic P-SV

$$S_{PS} = V_S S_P; \rho = a S_P^{-b}$$

$$\begin{cases} \lambda = \rho S_P^{-2} (1 - 2S_{PS}^2) = a S_P^{-b-2} (1 - 2S_{PS}^2) \\ \mu = \rho (S_{PS}/S_P)^2 = a S_P^{-b-2} S_{PS}^2 \\ \rho_0 = a S_P^{-b} \end{cases}$$

$$\begin{aligned} \nabla_{S_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial S_P} + \nabla_\mu \frac{\partial \mu}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P} \\ &= \nabla_\lambda a(-b-2) S_P^{-b-3} (1 - 2S_{PS}^2) \\ &\quad + \nabla_\mu a(-b-2) S_P^{-b-3} S_{PS}^2 + \nabla_{\rho_0} a(-b) S_P^{-b-1} \\ &= \left( \nabla_\lambda (b+2) (1 - 2S_{PS}^2) + \nabla_\mu (b+2) S_{PS}^2 + \nabla_{\rho_0} b S_P^2 \right) (-a) S_P^{-b-3} \\ \nabla_{S_{PS}} &= \nabla_\lambda \frac{\partial \lambda}{\partial S_{PS}} + \nabla_\mu \frac{\partial \mu}{\partial S_{PS}} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_{PS}} \\ &= \nabla_\lambda a S_P^{-b-2} (-4) S_{PS} + \nabla_\mu a S_P^{-b-2} 2 S_{PS} \\ &= (-\nabla_\lambda 2 + \nabla_\mu) 2 a S_P^{-b-2} S_{PS} \end{aligned} \tag{1}$$