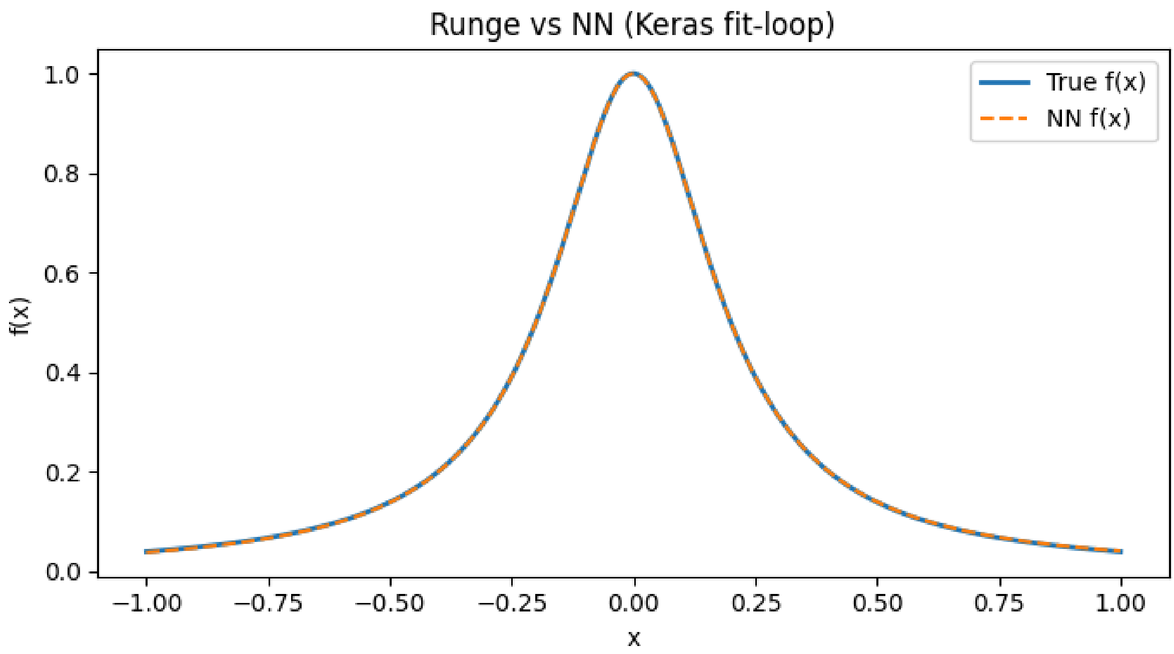
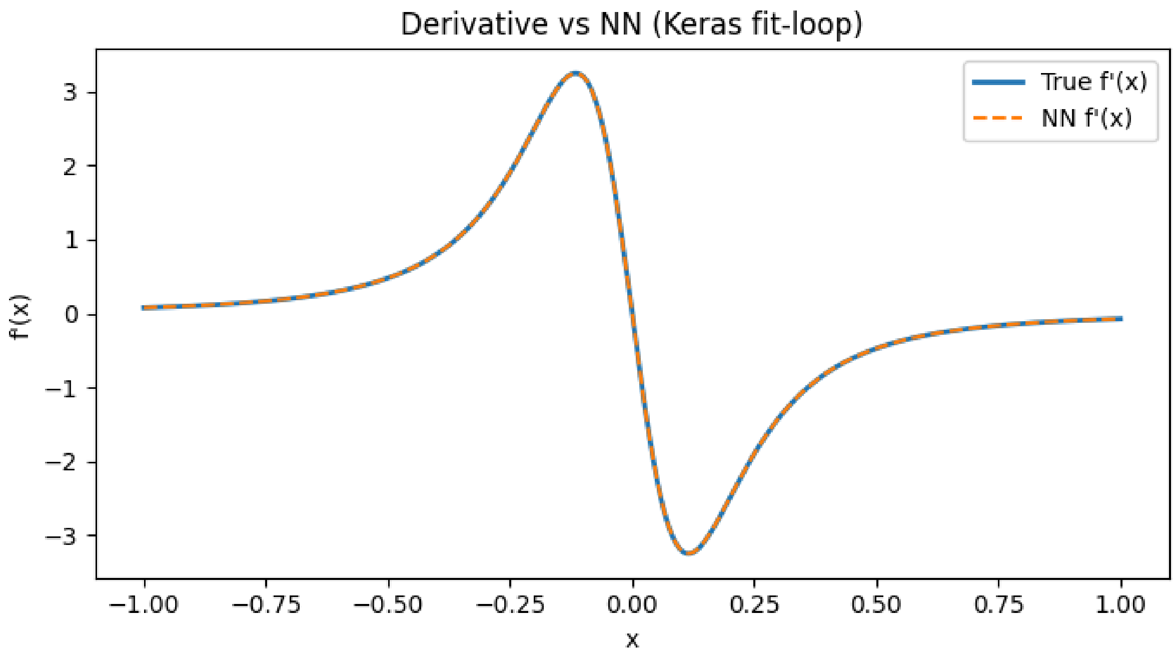
In [2]:
```
# === HW2 (Programming Assignment, minimal-diff version): Runge + derivative ===
import os, random
import numpy as np
import tensorflow as tf
import matplotlib.pyplot as plt

# ---------- reproducibility ----------
SEED = 12345
os.environ["PYTHONHASHSEED"] = str(SEED)
random.seed(SEED)
np.random.seed(SEED)
tf.random.set_seed(SEED)

# ---------- target function & derivative ----------
def runge_np(x):
    return 1.0 / (1.0 + 25.0 * x**2)

def drunge_np(x):
    return -50.0 * x / (1.0 + 25.0 * x**2) ** 2

# ---------- data ----------
rng = np.random.default_rng(SEED)
N_train, N_val = 2048, 512
X_train = rng.uniform(-1, 1, size=(N_train, 1)).astype(np.float32)
X_val   = rng.uniform(-1, 1, size=(N_val,   1)).astype(np.float32)

y_train  = runge_np(X_train).astype(np.float32)
dy_train = drunge_np(X_train).astype(np.float32)
y_val    = runge_np(X_val).astype(np.float32)
dy_val   = drunge_np(X_val).astype(np.float32)

train_ds = tf.data.Dataset.from_tensor_slices((X_train, (y_train, dy_train))).batch
val_ds   = tf.data.Dataset.from_tensor_slices((X_val,   (y_val,   dy_val))).batch(1

# ---------- minimal-change model (Sequential) ----------
def build_model(width=64, depth=2):
    layers = [tf.keras.layers.Input(shape=(1,))]
    for _ in range(depth):
        layers += [tf.keras.layers.Dense(width, activation="tanh")]
    layers += [tf.keras.layers.Dense(1, activation=None)]
    return tf.keras.Sequential(layers)

# ---------- wrap Sequential into a Model that also learns derivative ----------
class DerivModel(tf.keras.Model):
    def __init__(self, core, alpha=1.0, beta=1.0):
        super().__init__()
        self.core = core
        self.alpha = alpha
        self.beta = beta
        self.loss_tracker = tf.keras.metrics.Mean(name="loss")
        self.f_mse = tf.keras.metrics.Mean(name="mse_f")
        self.df_mse = tf.keras.metrics.Mean(name="mse_fprime")

    def call(self, x, training=False):
        return self.core(x, training=training)

    def train_step(self, data):
        x, (y_true, dy_true) = data
        with tf.GradientTape(persistent=True) as tape:
            tape.watch(x)  # 讓 Tape 追蹤輸入，才能對 x 求導
            y_pred = self.core(x, training=True)
            dy_pred = tape.gradient(y_pred, x)  # dy/dx
```

```
            loss_f  = tf.reduce_mean(tf.square(y_pred - y_true))
            loss_df = tf.reduce_mean(tf.square(dy_pred - dy_true))
            loss = self.alpha * loss_f + self.beta * loss_df
        grads = tape.gradient(loss, self.core.trainable_variables)
        self.optimizer.apply_gradients(zip(grads, self.core.trainable_variables))
        del tape

        self.loss_tracker.update_state(loss)
        self.f_mse.update_state(loss_f)
        self.df_mse.update_state(loss_df)
        return {"loss": self.loss_tracker.result(),
                "mse_f": self.f_mse.result(),
                "mse_fprime": self.df_mse.result()}

    def test_step(self, data):
        x, (y_true, dy_true) = data
        with tf.GradientTape() as tape:
            tape.watch(x)
            y_pred = self.core(x, training=False)
            dy_pred = tape.gradient(y_pred, x)
            loss_f  = tf.reduce_mean(tf.square(y_pred - y_true))
            loss_df = tf.reduce_mean(tf.square(dy_pred - dy_true))
            loss = self.alpha * loss_f + self.beta * loss_df

        self.loss_tracker.update_state(loss)
        self.f_mse.update_state(loss_f)
        self.df_mse.update_state(loss_df)
        return {"loss": self.loss_tracker.result(),
                "mse_f": self.f_mse.result(),
                "mse_fprime": self.df_mse.result()}

    @property
    def metrics(self):
        # 讓 model.reset_metrics() 正確運作
        return [self.loss_tracker, self.f_mse, self.df_mse]

# ---------- build/compile/fit (和你原本流程幾乎一樣) ----------
core = build_model(width=64, depth=2)
model = DerivModel(core, alpha=1.0, beta=1.0)  # 這裡可調權重
model.compile(optimizer=tf.keras.optimizers.Adam(1e-3))  # loss 內建於 train_step

history = model.fit(
    train_ds,
    validation_data=val_ds,
    epochs=1000,              # 依時間調整：1000~6000
    verbose=0                 # 想看過程就改成 1
)

# ---------- evaluate on dense grid ----------
x_test = np.linspace(-1, 1, 1001, dtype=np.float32).reshape(-1,1)
xT = tf.convert_to_tensor(x_test)
with tf.GradientTape() as tape:
    tape.watch(xT)
    y_hat_T = model(xT, training=False)
    dy_hat_T = tape.gradient(y_hat_T, xT)

y_hat  = y_hat_T.numpy()
dy_hat = dy_hat_T.numpy()
y_true  = runge_np(x_test)
dy_true = drunge_np(x_test)

def mse_np(a,b): return float(np.mean((a-b)**2))
def max_err(a,b): return float(np.max(np.abs(a-b)))
```

```python
print("\n=== Metrics (test grid) ===")
print("MSE f      :", mse_np(y_hat,  y_true))
print("MSE f'     :", mse_np(dy_hat, dy_true))
print("Max |err| f:", max_err(y_hat,  y_true))
print("Max |err| f':", max_err(dy_hat, dy_true))

# ---------- plots ----------
plt.figure(figsize=(7,4))
plt.plot(x_test, y_true, linewidth = 2, label="True f(x)")
plt.plot(x_test, y_hat, linestyle = "--",  label="NN f(x)")
plt.xlabel("x"); plt.ylabel("f(x)"); plt.title("Runge vs NN (Keras fit-loop)")
plt.legend()
plt.tight_layout()
plt.show()

plt.figure(figsize=(7,4))
plt.plot(x_test, dy_true, linewidth = 2, label="True f'(x)")
plt.plot(x_test, dy_hat, linestyle = "--",  label="NN f'(x)")
plt.xlabel("x"); plt.ylabel("f'(x)")
plt.title("Derivative vs NN (Keras fit-loop)")
plt.legend()
plt.tight_layout()
plt.show()

plt.figure(figsize=(7,4))
plt.plot(history.history["loss"], label="Train")
plt.plot(history.history["val_loss"], label="Val")
plt.xlabel("Epoch")
plt.ylabel("Loss  (α·MSE_f + β·MSE_f')")
plt.title("Training / Validation Loss")
plt.legend()
plt.tight_layout()
plt.show()
```

```
WARNING:tensorflow:Calling GradientTape.gradient on a persistent tape inside its c
ontext is significantly less efficient than calling it outside the context (it cau
ses the gradient ops to be recorded on the tape, leading to increased CPU and memo
ry usage). Only call GradientTape.gradient inside the context if you actually want
to trace the gradient in order to compute higher order derivatives.

=== Metrics (test grid) ===
MSE f      : 6.509344530059025e-07
MSE f'     : 4.824778443435207e-06
Max |err| f: 0.0013967528939247131
Max |err| f': 0.005621671676635742
```


Runge vs NN (Keras fit-loop)
True f(x)
NN f(x)
f(x)
x


Derivative vs NN (Keras fit-loop)
True f'(x)
NN f'(x)
f(x)
x


Training / Validation Loss
Train
Val
Loss (α·MSE_f + β·MSE_f')
Epoch

使用神經網路同時近似 Runge 函數與其一階導數

1) 目的（Purpose）

訓練一個一維神經網路 $f_\theta(x)$ ，**同時**近似：

- 函數值：$f(x) = \dfrac{1}{1+25x^2}$
- 導數：$f'(x) = \dfrac{-50x}{(1+25x^2)^2}$

為抑制只擬合函數值時的形狀偏差與邊界震盪，損失函數同時考慮值與導數： $$ \mathcal L(\theta) = \alpha \cdot \mathrm{MSE}\big(f_\theta(x),\, f(x)\big)

- \beta \cdot \mathrm{MSE}\big(\partial*x f*\theta(x),\, f'(x)\big). $$

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2) 假設函數（Hypothesis Function）

使用以 `tanh` 為非線性的全連接網路（兩層隱藏層），形式為

$$f_\theta(x) = W_3\ \tanh\Big(W_2\ \tanh(W_1 x + b_1) + b_2\Big) + b_3, \quad x \in \mathbb{R}.$$

$\partial_x f_\theta(x)$ 以 TensorFlow `GradientTape` 對輸入 x 求導得到。

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3) 資料抽樣（Data Sampling）

- **輸入分佈**：$x \sim \mathcal{U}[-1,1]$（均勻抽樣）。
- **資料量**：訓練集 $N_{\text{train}} = 2048$，驗證集 $N_{\text{val}} = 512$。
- **標註**：對每個 x 直接以解析式產生

$$y = f(x) = \frac{1}{1+25x^2}, \qquad y' = f'(x) = \frac{-50x}{(1+25x^2)^2}.$$

- **資料餵入**：`tf.data.Dataset` 以 `(x, (y, y'))` 的 tuple 形式傳入模型。

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4) 模型架構（Model Architecture）

- **型式**：`tf.keras.Sequential`
- **結構**：
  - Input：shape = `(1,)`
  - Dense(width=64, activation= `tanh`)
  - Dense(width=64, activation= `tanh`)
  - Dense(1, activation=None)（線性輸出）
- **導數計算**：在 `train_step` ／ `test_step` 以 `GradientTape` 對輸入 x 求 $\partial_x f_\theta(x)$ 並納入損失。

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5) 訓練設定與參數（Hyperparameters & Training Setup）

- **損失權重**：$\alpha = 1.0$、$\beta = 1.0$
  （導數擬合不足可調大 β 至 2–5。）
- **最佳化器**：Adam，學習率 1×10^{-3}。
- **批次大小**：train = 64；val = 128。
- **訓練回合**：`epochs = 1000`。
- **隨機種子**：全域固定為 12345 以利重現。
- **評估**：在等距測試網格 $x \in [-1, 1]$（例如 1001 點）計算 $\mathrm{MSE}_f = \mathrm{MSE}(f_\theta, f)$、$\mathrm{MSE}_{f'} = \mathrm{MSE}(\partial_x f_\theta, f')$，並回報最大絕對誤差。

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6) 結果（Results）

> 附圖（來自執行程式碼）：
>
> 1. 真實 $f(x)$ 與 NN $f_\theta(x)$ 疊圖。
> 2. 真實 $f'(x)$ 與 NN $\partial_x f_\theta(x)$ 疊圖。
> 3. 訓練／驗證損失曲線（$\alpha \cdot \mathrm{MSE}_f + \beta \cdot \mathrm{MSE}_{f'}$）。

請填入實際執行輸出的數值（或保留由程式自動列印）：

指標	數值
Test MSE f	6.509344530059025e-07
Test MSE f'	4.824778443435207e-06
Max $\lvert f_\theta - f\rvert$	0.0013967528939247131
Max $\lvert\partial_x f_\theta - f'\rvert$	0.005621671676635742

由圖片與MSE的數值可以知道，目前所使用的模型可以成功的擬合$f(x)$跟$f'(x)$
